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Case study

A hybrid strategy of AutoML and SHAP for automated and explainable concrete strength prediction

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ABSTRACT

The precise prediction of concrete compressive strength is essential for ensuring safe and reliable infrastructure design and construction. However, traditional empirical models often struggle to accurately predict compressive strength due to the complex nonlinear relationship between concrete properties and target strength. This study introduces an AutoML-SHAP (Automatic Machine Learning - SHapley Additive exPlanations) strategy, designed to automatically predict the compressive strength of concrete and provide insightful interpretations of the predictive outcomes. The AutoML model uses K-fold bagging and multilayer stacking to automate model selection and hyperparameter tuning. The integration of AutoML and SHAP offers synergistic benefits, facilitating the development of a precise, efficient, and comprehensively interpretable model. Results demonstrate that AutoML-SHAP model outperforms other machine learning models for predicting compressive strength without human intervention. The AutoML model is automatically established within 174 s and exhibits comparable predictive performance with $R^2 = 0.96$, RMSE = 3.63, and MAE = 2.41. SHAP provides a global explanation of the impact of mixing parameters on compressive strength, and a local explanation of feature contribution to each prediction, making the process transparent and reliable. Feature dependence analysis reveals the influence tendency of mixing parameters on strength.

1. Introduction

The construction of safe and dependable infrastructure is a crucial challenge confronting societies worldwide. Accurately predicting the compressive strength of concrete is essential for designing and constructing safe and reliable infrastructure. Nevertheless, predicting concrete strength is a complex undertaking due to the numerous variables that impact compressive strength. Traditionally, two methods have been employed to determine concrete strength: field testing and empirical model calculations. Field testing frequently necessitates retaining test specimens during concrete pouring or coring on the hardened concrete structure prior to strength testing. It provides the most accurate strength, but it is a cumbersome and laborious process that can lead to defective structures.

An alternative method to obtain concrete strength is to use mathematically empirical models [1,2]. This approach requires

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pre-calibration of the selected model to determine the values of the associated parameters. However, the calibration process is tedious and requires testing of compressive strength. Additionally, mathematical modeling methods are limited in their application due to the need for multiple corrections for different mixes and the complexity of the calibration process. Many factors influence the compressive strength of concrete, including the type and amount of cement, the water-to-cement ratio, the size of aggregates (both fine and coarse), as well as the type of chemical admixtures used [3]. Achieving the desired strength in concrete requires meticulous regulation of multiple factors, and the interaction between various raw materials can significantly affect the compressive strength of concrete. Furthermore, non-linear strength development can occur depending on the mixture's composition and exposure conditions, which further complicates the prediction of compressive strength [4,5]. Therefore, it is crucial to consider all of these factors when predicting the compressive strength of a material [6,7]. Novel methods that offer high prediction accuracy and simple operational processes are eagerly anticipated.

Machine learning (ML) models can be trained using datasets that contain input and output variables, allowing them to learn the relationship between these variables without being limited by pre-existing intuitive understanding. These models can analyze vast amounts of data and identify complex patterns and relationships that may not have been apparent to human observers. This ability to recognize and learn from these patterns is a key feature of ML, enabling more accurate predictions and insights in a wide range of fields. In civil engineering, ML's ability to capture complex non-linear relationships between inputs and predictions has made it popular for developing prediction models in various areas, such as structural health monitoring [8], performance prediction [9–11], and modeling of mechanical behavior [12–14], among others. There are various ML methods available, including support vector machines (SVM), artificial neural networks (ANN), multiple linear regression (MLR), decision trees (DTs), random forests (RF), and extreme gradient boosting (XGBoost), each utilizing different algorithms and techniques to solve different types of problems [15–19]. These methods have shown effectiveness in addressing a wide range of challenges, from predictive modeling to data analysis and decision-making processes. As ML continues to advance, researchers are constantly seeking new ways to enhance the performance of ML algorithms. However, deploying high-performance ML models poses two significant challenges: model selection and hyperparameter optimization. Model selection involves choosing the appropriate ML algorithm for a specific dataset, and it is a critical stage in the ML process. Selecting the appropriate ML algorithm for a particular dataset can be challenging, but it is a crucial stage in the machine learning process.

In general, it is challenging to identify an ML algorithm that performs superbly across the board. Therefore, several ML techniques are used to develop prediction models for a particular dataset, and the final model is then chosen among those with the best performance [11,20]. Hyperparameters are values that are set prior to training the model, and they can significantly impact the performance of the model. Hyperparameter optimization involves selecting the optimal values for these parameters to achieve the best performance of the model. This process can be challenging and time-consuming, as there are typically many possible combinations of hyperparameters to consider. There are several techniques available for optimizing hyperparameters in machine learning models, such as grid search, random search, and Bayesian optimization [21,22]. However, the process of tuning multiple hyperparameters can often be complex and time-consuming, leading to significant challenges and delays in the modeling process. The increasing complexity of data and the need for more accurate models has led to the emergence of Automated Machine Learning (AutoML) as a rapidly growing field. AutoML seeks to automate the process of implementing high-performance ML models and hyperparameter optimization on a given dataset, reducing the need for manual intervention and improving the efficiency of model development and deployment. Despite its potential advantages, there is currently a lack of research on the application of AutoML in civil engineering. However, some studies have reported the successful use of AutoML in identifying damage and susceptibility to landslides [23–25], demonstrating its potential in this field. Furthermore, in predicting the compressive strength of concrete, which is influenced by multiple mixing factors, AutoML has enormous potential and warrants further exploration.

While AutoML has the potential to deliver highly accurate predictions, the complexity of the resulting models can make it challenging to interpret the contribution of each input variable to the model's output. This lack of interpretability can limit the practical application of these models in fields where transparency and explainability are essential. To address this issue, recent developments in machine learning have focused on developing models that can elucidate the relationship between input variables and predicted results [26]. SHapley Additive exPlanations (SHAP) is one such model that has been developed to explain the impact of individual input variables on the output of a machine learning model. By analyzing the contribution of each input variable to the model's output, SHAP can identify the key drivers of the model's predictions and provide insights into the underlying factors that influence the output [27,28]. By integrating SHAP with AutoML, it is possible to develop an accurate, automated, and interpretable ML strategy for predicting the compressive strength of concrete. This approach can enable civil engineers to develop more accurate and efficient models for use in a range of applications, including structural design and analysis, risk assessment, and decision-making.

2. Research significance

This study proposes an AutoML-SHAP strategy for predicting the compressive strength of concrete, which can effectively interpret the predicted outcome from global feature importance to the contributions of each parameter in a specific specimen. AutoML enhances the accessibility and efficiency of the predictive model by achieving high performance in various ML problems without human intervention, including data pre-processing, feature engineering, model selection, and hyperparameter tuning. By integrating the AutoML model with SHAP, the proposed model becomes interpretable, allowing for a better understanding of the model's accurate output. This investigation further provides insights into the interaction of the mixing parameters on the compressive strength of concrete by using SHAP to provide global, local, and feature-dependent explanations. This approach offers a comprehensive understanding of the relationships between input variables and predicted outcome concrete compressive strength, improving the practical applicability of machine learning models in concrete technology. The development of an accurate, automated, and interpretable ML strategy has significant potential to advance the field of civil engineering and contribute to the development of more effective and efficient solutions for a range of challenges. As such, ongoing research in this area is essential to further advance the field and drive innovation in this critical area of engineering.

3. Methodology

3.1. Automated machine learning

State-of-the-art ML techniques are growing more sophisticated, making it increasingly challenging even for ML experts to incorporate all the latest best practices into modeling. To address this problem, the AutoML strategy based on the AutoGluon framework is adopted in this study for concrete compressive strength prediction [29]. AutoML processes heterogeneous datasets robustly and utilizes model assembly process that combines repetitive K-fold bagging and multi-layer stacking. Among the multilayer stacking, base ML models are included in the lower layer and the outputs are combined with the origin features to provide the input features for the higher layer. Furthermore, the repeated K-fold bagging approach is used to improve the stacking performance and reduce overfitting. The K-fold bagging includes randomly partitioning the data into K distinct subsets, followed by training K copies of the model with different K-1 subsets kept out of each copy. In this approach, every iteration of the model is tasked with generating out-of-fold (OOF) predictions on the validation subset. Subsequently, the higher-level models are trained solely on the lower-level OOF predictions. This methodology enables the model to improve its predictive accuracy and mitigate overfitting by preventing the information leakages that arise from incorporating the training data in the validation process.

The AutoML strategy usually uses a combination of transfer learning and reinforcement learning to automatically train models for prediction. Transfer learning is about utilizing prior knowledge or models to enhance learning and performance on related tasks, while reinforcement learning focuses on automating decision-making processes in AutoML through trial and error to maximize cumulative rewards. Both techniques contribute to the advancement of AutoML by improving efficiency, generalization, and performance of machine learning models in different ways. In this study, to avoid algorithm selection and hyperparameter optimization, the AutoML

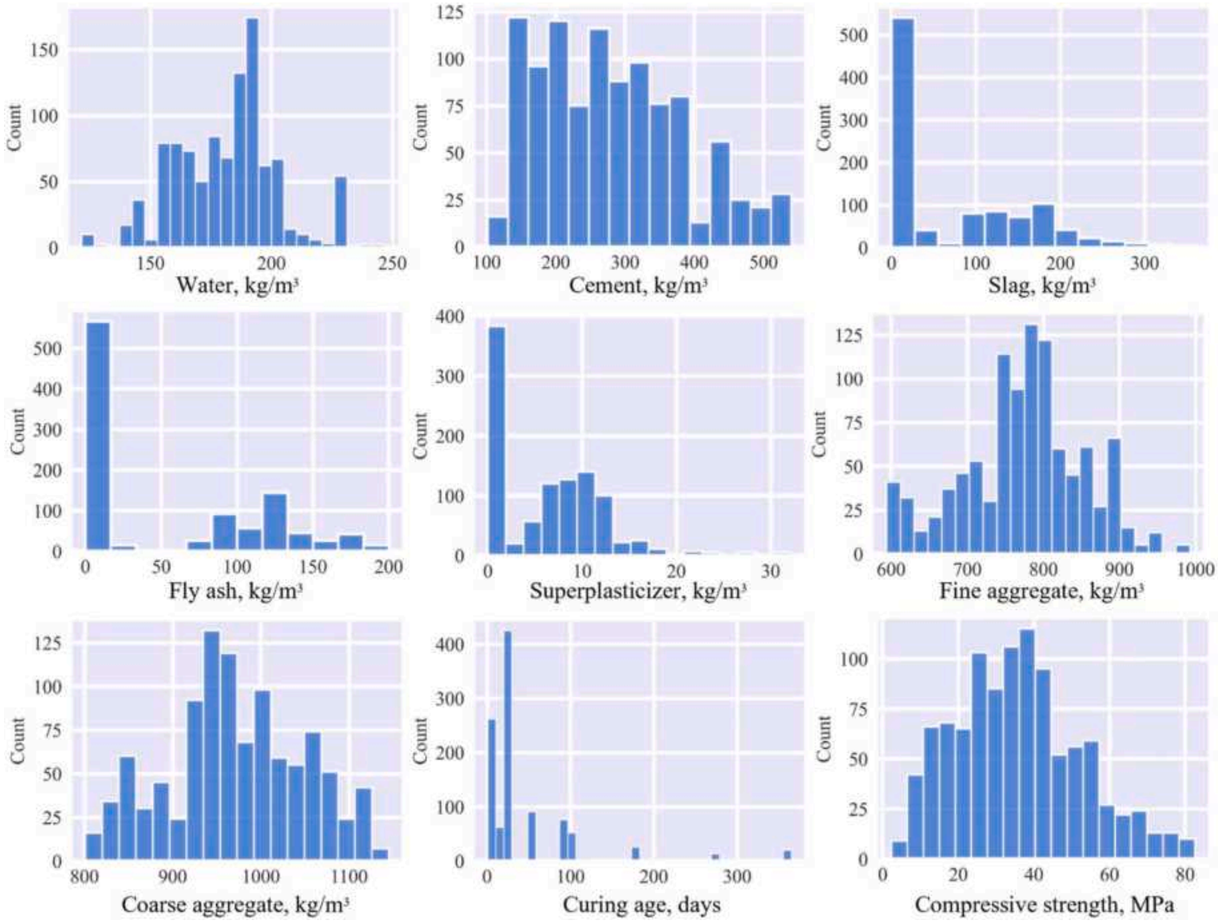


Fig. 1. Detailed distribution of variables in the dataset.

model simply reuses all base ML models as the stacking model and utilizes the same hyperparameter values for all models. Furthermore, the structure of the AutoML model is automatically tuned based on the given or default search time. This study demonstrates the feasibility of the AutoML strategy for training models for the task of predicting the compressive strength of concrete. As for the base ML models, random forest (RF), k-nearest neighbors (KNN), CatBoost boosted trees (CatBoost), LightGBM boosted trees (LightGBM), extreme gradient boosting (XGBoost), extra trees (ET), and neural networks (NN) are among the customizable models used in the AutoML model. Since the base ML models applied have already been widely applied [11,18,21,30,31], the models are not further introduced in this study.

3.2. SHapley Additive exPlanations (SHAP)

The SHAP model, proposed by Lundberg and Lee in 2017 [27], is a mathematical technique that elucidates the outputs of machine learning models. This method provides a means to interpret the impact of individual input features on the predicted output, making it particularly useful for explaining complex models. The SHAP method, which is rooted in game theory, is premised on the notion that every feature in the input data contributes to the prediction generated by the model. The contribution of each feature can be measured by its Shapley value, which is a measure of the feature's importance in relation to the other features in the model. This approach provides a rigorous framework for understanding how each feature affects the output, and it has been shown to be effective in explaining the behavior of complex machine learning models [28,32].

4. Database engineering and performance measures

4.1. Database

To develop machine learning models, a dataset consisting of 1030 concrete compressive strength test results was employed. The data, which was collected by Yeh [33,34] and obtained from the UCI ML Repository, has been previously utilized to train and evaluate a range of machine learning algorithms [21,35–37]. There are eight independent features included in the dataset, specifically Ordinary Portland cement, water, fly ash, superplasticizer, slag, fine and coarse aggregate, and curing age. The concrete compressive strength is the dependent variable that serves as the output. The distribution of each feature in the dataset is presented in Fig. 1. The Statistics of variables are illustrated in Table 1. The histograms indicate that Portland cement, water, coarse aggregate, fine aggregate, and compressive strength predominantly follow Gaussian distributions. Expanding the feature distribution range can potentially enhance the generalization ability of the machine learning model. This broader range of feature distributions can help the model predict the compressive strength of different concrete components more effectively. Pearson correlation coefficient of variables in the dataset are shown in Fig. 2. Based on the Pearson correlation coefficients, it can be observed that there is a generally weak linear correlation among the majority of variables. This suggests that the non-linear machine learning model employed in this study is more effective on concrete compressive strength prediction. The application of these models enable a better capture of the non-linear relationships between variables, thereby enhancing the predictive capability for concrete compressive strength.

4.2. Performance measures

Three metrics, correlation of determination (R2), root mean squared error (RMSE) and mean absolute error (MAE), were utilized to assess the performance of the prediction algorithms. R^2 indicates the linear correlation between the predicted and actual results, with a range of values from zero to one. A higher value of R^2 indicates better performance of the prediction model. The RMSE is defined as the square root of the mean square error and quantifies the discrepancy between the predicted and actual values. Similarly, MAE is a statistical measure that gauges the accuracy of the prediction model by calculating the mean of the absolute difference between the predicted and actual values. The performance of the prediction method is deemed better with lower values of both RMSE and MAE. The three performance measures are summarized as follows:

Correlation of determination (R^2)

Table 1
Statistics of variables in the dataset.

	Unit	Mean	St.D.	Min.	Med.	Max.
OPC	kg/m^3	281.17	104.51	102.00	272.90	540.00
FA	kg/m^3	54.19	64.00	0.00	0.00	200.10
BFS	kg/m^3	73.90	86.28	0.00	22.00	359.40
Water	kg/m^3	181.57	21.36	121.75	185.00	247.00
SP	kg/m^3	6.20	5.97	0.00	6.35	32.20
CA	kg/m^3	972.92	77.75	801.00	968.00	1145.00
FA	kg/m^3	773.58	80.18	594.00	779.51	992.60
Age	days	45.66	63.17	1.00	28.00	365.00
Strength	MPa	35.82	16.71	2.33	34.44	82.60

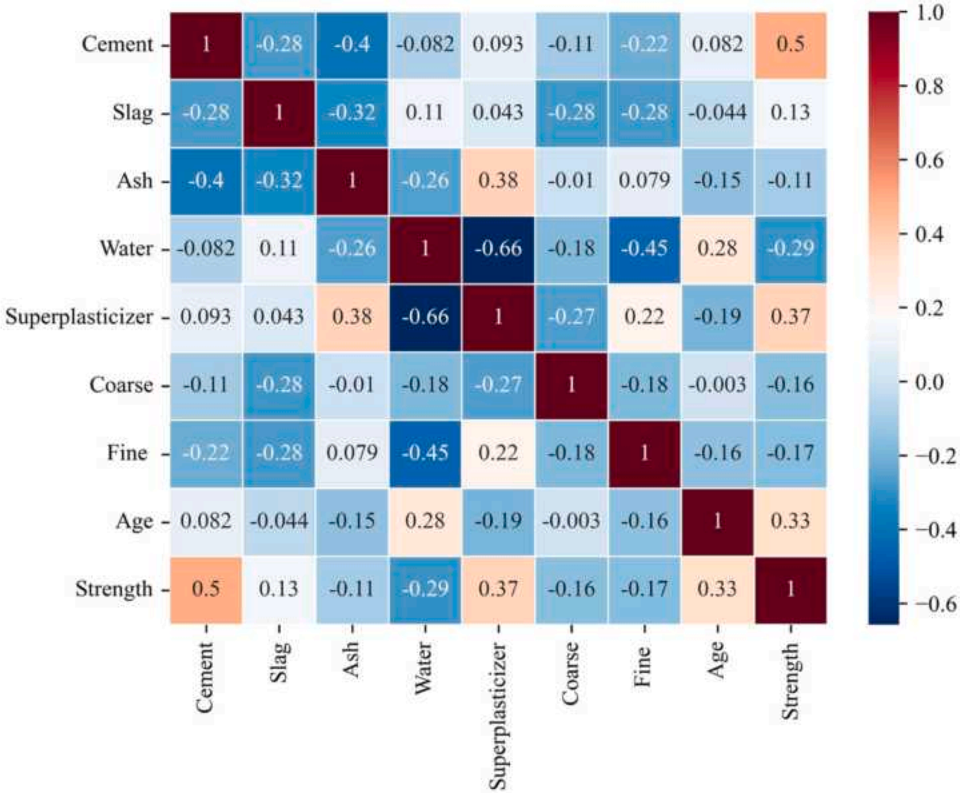


Fig. 2. Pearson correlation coefficient of variables in the dataset.

$$R^2 = 1 - \frac{\sum_{i=1}^{j} (P_i - T_i)^2}{\sum_{i=1}^{j} (T_i - \overline{T})^2} \tag{1}$$

Root mean squared error (RMSE)

$$RMSE = \sqrt{\frac{\sum_{i=1}^{j} (P_i - T_i)^2}{j}} \tag{2}$$

Mean Absolute Error (MAE)

$$MAE = \frac{\sum_{i-1}^{j} |P_i - T_i|}{j} \tag{3}$$

where, T_i and P_i represent the actual value and predicted value, respectively; $\overline{T}$ represents the mean actual value; j represents the sample numbers.

The data is partitioned into two sets, with 80 % of the dataset dedicated to training the model, and the remaining 20 % set aside for evaluating the model's predictive accuracy. To enhance the model performance, a 5-fold cross-validation is utilized during the training process. Subsequently, a comparison is made between the predictive performance of the AutoML model and traditional ML models.

5. Implementation of the AutoML model

Traditional ML models require complicated modeling procedures, such as data preprocessing, feature engineering, data splitting, hyperparameter tuning, model selection strategies, among others. The primary focus of most endeavors aimed at mitigating this issue has been on the combined selection of algorithms and optimization of hyperparameters. These efforts offer strategies for identifying the optimal model and its hyperparameters from an extensive set of possibilities. However, the brute-force search wastes significant computing resources by evaluating configurations of models and hyperparameters that are irrelevant to the specific domain. AutoML is able to establish a high-performance model automatically without ML expertise and the tedious process. Fig. 3 illustrates the modeling procedures that involve manual intervention in traditional ML models and AutoML. It can be seen that only the feature engineering process in AutoML needs to be performed manually according to the requirements. All other procedures are carried out automatically and require no manual intervention at all.

The only hyperparameter that should be emphasized for the AutoML modeling is the training time. Assuming adequate training time, AutoML performs the k-fold bagging procedure on k distinct and randomly selected partitions of the training data, subsequently averaging all out-of-fold (OOF) predictions across the repeated bags. The default training time is to ensure that all base models have completed the training, but not repeatedly. In our experiments, the default training time (training for one round) is 200 s. In the 5-fold cross-validation, the R^2 of validation set reaches the peak value of 0.9401 at 174 s. This means that the AutoML predictive model for the concrete compressive strength with the default training time is automatically established without manually tuning the hyper-parameters. Researchers in the engineering domain can quickly implement an AutoML model within the AutoML framework instead of manually selecting ML algorithms and tuning hyperparameters, allowing them to devote more time to the domain problem.

6. Model prediction performance

6.1. Comparison of model predictions

Table 2 lists the prediction performance metrics between the AutoML model and other base ML models. The results show that AutoML outperforms other base ML models in terms of accuracy. The AutoML model obtained the highest R^2 value with 0.96, slightly higher than CatBoost's 0.95. Except for KNN, all other ML models had R^2 greater than 0.9. This is because KNN is a single model,

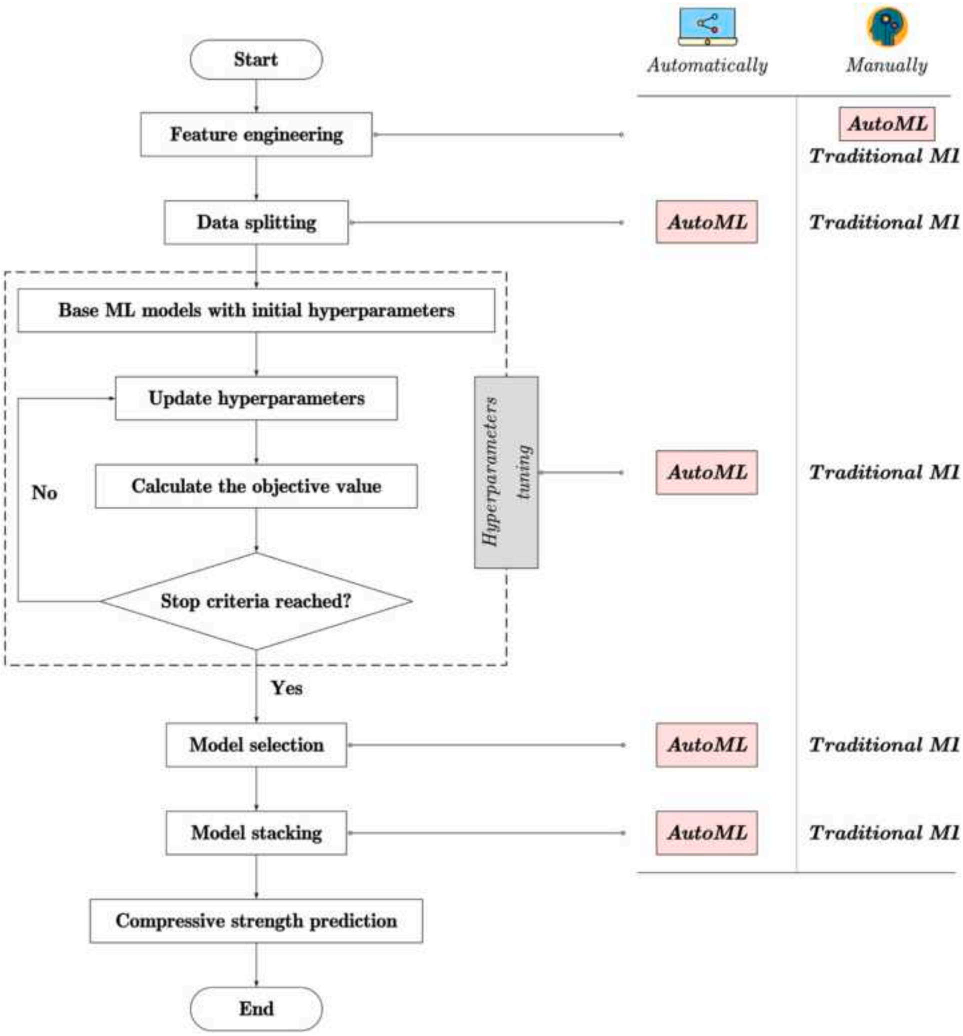


Fig. 3. Modeling procedures and comparison of AutoML and traditional ML methods.

Table 2
Prediction performance of applied ML models.

	R^2	RMSE	MAE	Standard error
AutoML	0.96	3.63	2.41	0.12
CatBoost	0.95	3.82	2.47	0.13
NN	0.94	4.05	2.87	0.13
GBM	0.94	4.27	2.76	0.14
XGBoost	0.94	4.35	2.87	0.14
ET	0.93	4.58	3.32	0.14
RF	0.92	4.89	3.50	0.16
KNN	0.80	7.68	5.10	0.25

whereas all other models are ensemble models, and the prediction accuracy of a single model often lags behind the ensemble model. Similarly, the RMSE and MAE values of AutoML are both lower than other base ML models, demonstrating its lower error values in prediction. In the case of the standard error value of the model, it was found that the AutoML model obtained the smallest dispersion of the prediction error with 0.12. As expected, KNN gets the maximum standard error of 0.25. According to the results, the ensemble model AutoML is effective in reducing the bias and variance of the base models through the ensemble strategy. This greatly improves the accuracy and reliability of AutoML in compressive strength prediction and indicates that AutoML is a promising tool for predictive modeling.

6.2. Model error analysis

Regarding the dispersion of the prediction outcomes, the AutoML model displays the narrowest IQR, whereas the KNN model demonstrates the greatest dispersion. Although the Catboost model has an IQR similar to that of the AutoML model, a larger outlier can be found. The models of AutoML, CatBoost, GBM, and XGBoost, demonstrate mean and median error values that are remarkably similar to the ideal prediction of 1.0, which suggests that these models have low prediction bias.

Fig. 4 illustrates the error distribution of the applied ML models. The interquartile range (IQR) of the mean and median values of the model error are presented, alongside any outliers, which are data points exceeding 1.5 times the IQR. With respect to the dispersion of the prediction outcomes, the AutoML model displays the narrowest IQR, indicating the greatest consistency among the prediction results. Conversely, the KNN model demonstrates the largest dispersion, which implies that its prediction outcomes exhibit a greater degree of variability. While the Catboost model has a similar IQR to the AutoML model, it has a larger outlier, suggesting that it has a higher propensity for error in some instances. Notably, the AutoML, CatBoost, GBM, and XGBoost models demonstrate mean and median error values that are remarkably close to the ideal prediction of 1.0, indicating that these models have low prediction bias. The results suggest that the ML models utilized in the study perform well, with the AutoML model demonstrating the greatest consistency among the models. The error distribution of the models is well-distributed across the range of predictions, which is an important factor in ensuring that the models are reliable and effective.

To visually showcase the precision of the prediction, Fig. 5 presents the scatter plots of the predicted and actual compressive

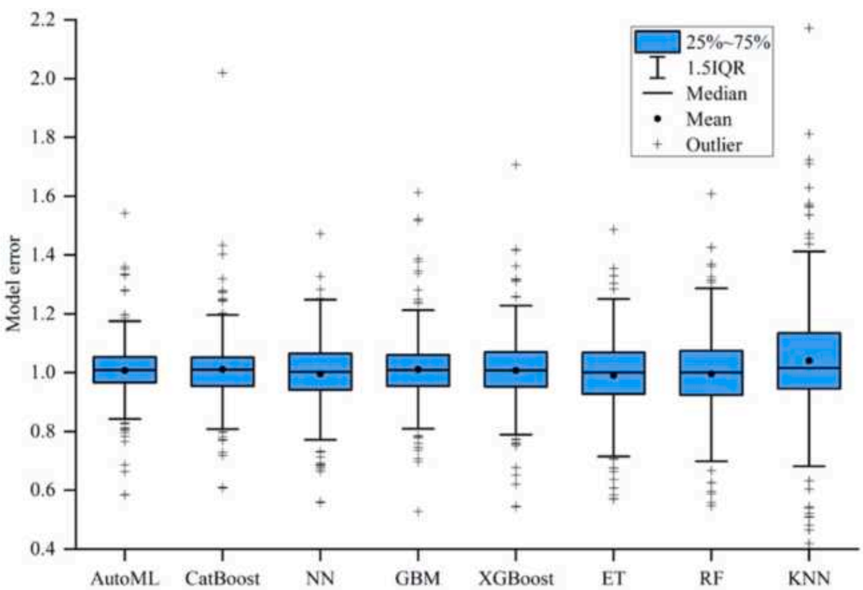


Fig. 4. Distribution of prediction error of the applied ML models.

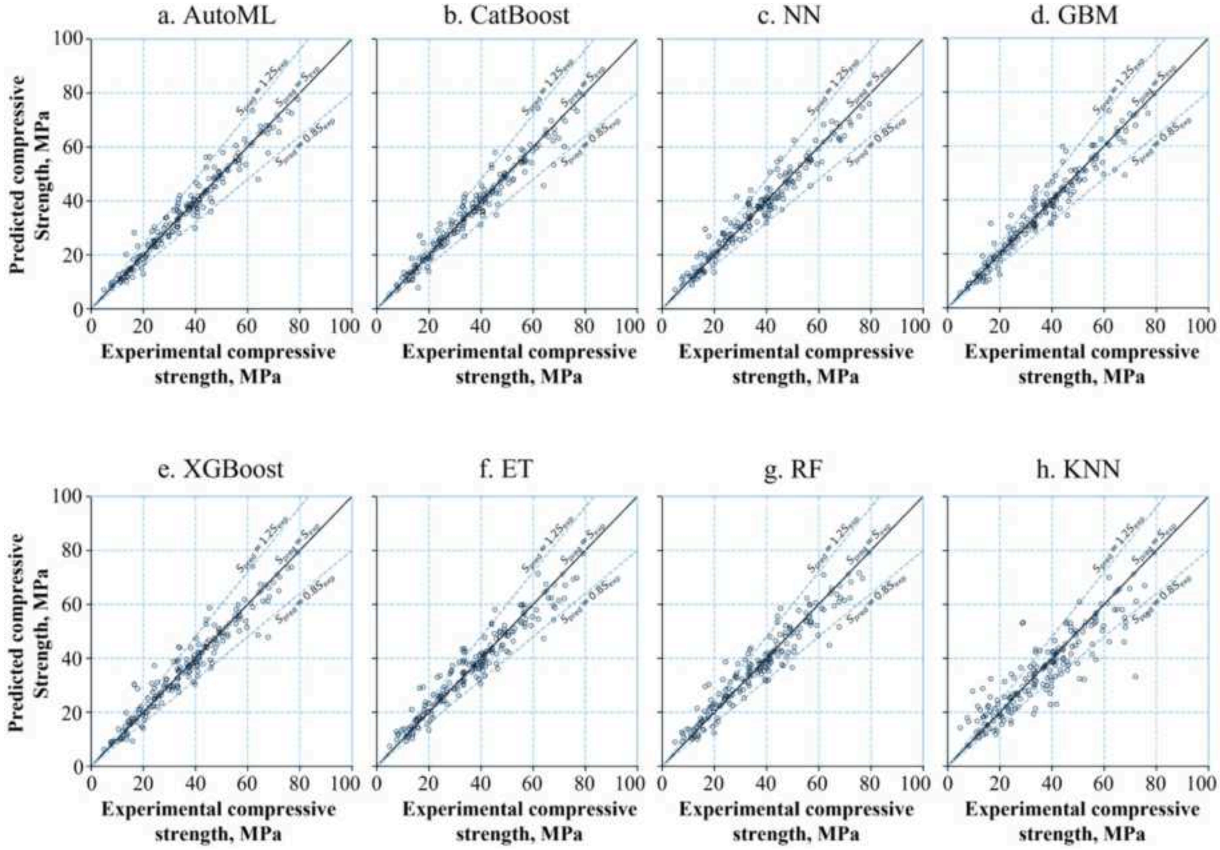


Fig. 5. Scatter plots of the predicted and actual compressive strength.

strength using the AutoML model and other base ML models. The consistency between the predicted and experimental values of the different models was evaluated, and it was found that the AutoML model outperformed the other models with greater overlap of the scatter with the y = x line and fewer scatters outside the 20 % error range. Moreover, the AutoML model demonstrated sufficient precision in predicting compressive strength within 20 MPa, and other integrated ML models such as CatBoost, NN, GBM, and XGBoost likewise exhibited competitive predictive performance over the entire range of compressive strengths. However, the remaining base models showed weaker predictive performance with scattered predictive values over the experimental values.

The AutoML model's simplicity of operation and timeliness provide additional advantages, demonstrating its great potential in practical applications. Therefore, the AutoML model may be a promising tool for predicting compressive strength in various fields, such as civil engineering and materials science. Despite the the AutoML model has demonstrated promising results, it is important to consider its generalization capability to other datasets, which requires further investigation in future research. Additionally, the

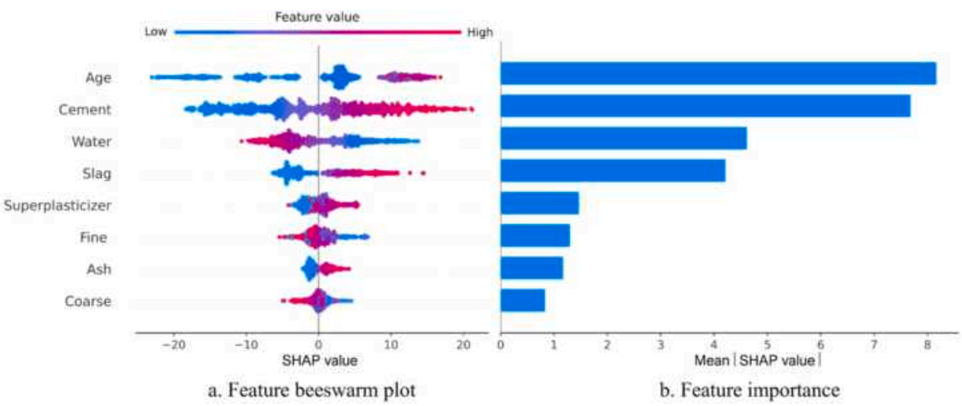


Fig. 6. Feature importance ranking based on SHAP value.

interpretation of the model's predictions and the underlying mechanisms of its superior performance should be explored to gain a deeper understanding of the predictive ability of AutoML model.

7. Explanation of the prediction based on AutoML-SHAP

7.1. Global explanation

There are multiple built-in importance type alternatives for the same ML model, but different techniques to output feature importance are available for most tree-based models. The process of model selection is often not well-documented and heavily reliant on the experiences and expertise of researchers. The importance ranking could change significantly depending on the number of factors. In contrast, SHAP values provide a more accurate assessment of causal inference, consistently identify significant features, and are better at identifying influential factors. Therefore, the SHAP values represent the impact of the feature on the model output, and the average absolute SHAP value can be ranked as a basis for analyzing the feature importance ranking [27]. The effect of each feature on the output of the model is provided by SHAP, allowing insight into which features are the most important to the model, as shown in Fig. 6. The ascending order of importance of the input parameters is depicted on the y-axis of Fig. 6a. Each point on the plot is colored according to its corresponding SHAP value, with blue indicating low values and red indicating high values. The density indicates the concentration of data points with particular SHAP value. Fig. 6a demonstrates that the curing age is the most important parameter, having an increasing positive and considerable influence on the output of compressive strength.

The results indicate that the age of curing is the most important factor affecting compressive strength, with a positive correlation observed between age and strength. Similarly, cement is found to have a significant positive impact on compressive strength. Conversely, the water-binder ratio was found to have a negative effect on compressive strength, with an increase in mixing water resulting in a decrease in strength, which is consistent with the conventional understanding. It can be found that the amount of cement and water, as well as the age of curing, are the most critical factors determining the strength of concrete. The significance of these factors on concrete strength is well-established in literatures [38,39]. The water-to-cement ratio is known to be a critical factor in the strength of concrete, as it affects the hydration of cement. Similarly, the age of curing is also widely recognized as an essential parameter in determining concrete strength, as the continued curing allows for further hydration and strength gain. While the remaining mineral admixtures and chemical additives have a relatively minor impact on strength, they still contribute to the overall prediction accuracy of the ML model. The global explanation of importance provides valuable insights into the key factors that affect concrete strength, which can inform the optimization of concrete mix design for enhanced performance. Further research could explore the interaction between these factors and their impact on other properties of concrete, such as durability and workability.

In Fig. 7, a heatmap is presented to provide comparable explanations for the model output based on hierarchical clustering. The instance indices are on the x-axis, with the model inputs on the y-axis, and the SHAP values encoded on a color scale. The upper subfigure displays the prediction value, denoted by the black curve $f(x)$, while the gray dashed line represents the average value. Fig. 6 specifically focuses on illustrating the distributions of SHAP values for different features within the dataset, as well as the distributions of SHAP values across different samples. The key factor influencing compressive strength, curing age, has a detrimental effect on the output for the instances between 400 and 500, resulting in the output value f(x) is below average within this range. And around the 1000_{th} instance, the main impact features (age, cement, water, and slag) all exhibit favorable effects, leading to higher prediction values. By revealing the internal structure of the ML model with minimal artificial intervention, SHAP provides a comprehensive explanation of the basic principles of prediction underlying the entire prediction results. As a result, it can effectively facilitate the interpretation of the impact of mixing parameters on the concrete compressive strength without significant effort.

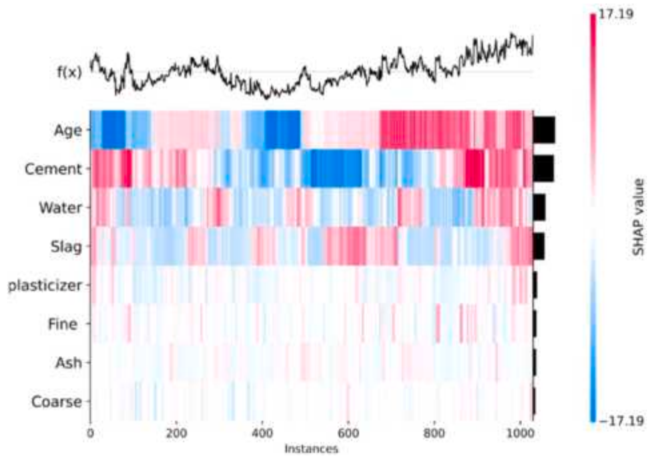


Fig. 7. Overall importance of input features.

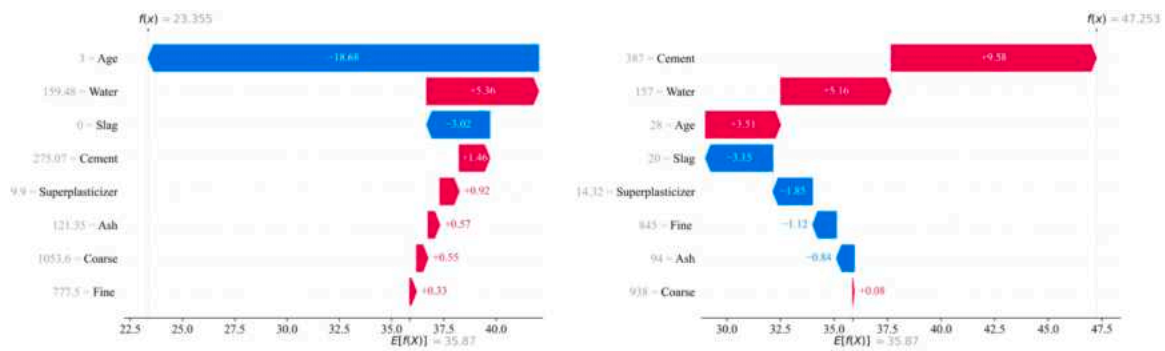
7.2. Local explanation

SHAP can also provide a local explanation for each individual prediction, which can be particularly useful in understanding the impact of specific features on the prediction. Two instances of local explanation for compressive strength prediction are illustrated in Fig. 8 using a waterfall plot. Each arrow in the figure denotes the direction and size of the influence of a feature on the prediction. The plot begins with the average of the output values $E[f(x)]$ at the bottom. According to the principle of linear additivity, the outcome of each feature's contribution is added together to provide the final prediction. A comparison of the two figures reveals some interesting contrasts. A curing age of 28 days has a beneficial effect, while a curing age of 3 days has a considerable negative influence on the output of compressive strength. This negative influence is based on the entire dataset in terms of the output results for compressive strength. In other words, the SHAP values for a curing period of 28 days exceed the average SHAP value, whereas for a curing period of 3 days, the SHAP values fall below the average. This means that a longer curing time contributes to the development and maturity of concrete strength. Similarly, a higher amount of cement has a clear positive effect on compressive strength, as identified by SHAP in Fig. 8b. These local explanations provide valuable insights into the specific factors that influence concrete strength prediction. For both instances, the water mixing is relatively close, and it can be seen that their contributions to the predicted outputs are likewise close.

The local explanation of SHAP enables an intuitive understanding of the role of each feature in each prediction, thus making the prediction process transparent. This allows us to see which features are most important in each prediction and how they contribute to the overall prediction. In addition, the local explanation of SHAP can serve to explain the origin of a particular prediction, and to identify any potential errors in the prediction process. The local explanation of SHAP also allows the incorporation of feedback data into the prediction process, which can improve the accuracy of the predictions.

7.3. Interdependence explanation

The process of generating compressive strength in concrete is a highly complex process that involves the interaction of various mixed raw materials. However, the SHAP method offers a valuable tool to quantify the dependence of different features and provides insight into how each mixing parameter affects compressive strength. Fig. 9 illustrates this by presenting three representative groups of feature dependence plots. These plots show the relationship between the predicted output and individual features while accounting for the effects of other features. Such an approach is useful in revealing the non-linear relationships between features and compressive strength output, helping to identify the most critical mixing parameters that affect the outcome. As shown in Fig. 9a, the SHAP value exhibits a rapid increase that slows down as the curing age increases, regardless of the amount of cement mixing. This is in agreement with our knowledge on the growth of concrete compressive strength, where early-age cement hydration drives rapid growth in compressive strength, slowing down after a certain age is reached [40]. The dependence of the superplasticizer and water on the compressive strength output is shown in Fig. 9b. The addition of superplasticizer enhances its positive contribution to compressive strength. However, this contribution is not linear and reaches a limiting point slightly above 10 kg/m^3 before decreasing slightly or remaining constant. Conversely, the addition of superplasticizer significantly reduces the amount of water blended into the concrete. According to Fig. 9c, the contribution of cement to compressive strength demonstrates a linear relationship. As more cement is added, the compressive strength increases progressively. The mixing of superplasticizers did not seem to change this trend, but increased the slope of the linear relationship, implying an acceleration of the strength growth. At low levels of cement mix (less than 200 kg/m^3), the incorporation of superplasticizers reduces the contribution of cement to compressive strength or decreases compressive strength. When the amount of cement mixing is between 300 and 500 kg/m^3, the superplasticizer mixture increases the compressive strength. The feature dependence analysis of SHAP allows for a better understanding of the relationships between features and their contribution to the output results. By examining how certain features interact with each other, it is possible to better understand how each feature contributes to the overall output. This information can be helpful in making informed decisions about which features to include in a plan, and in determining which features are most important for achieving the desired results. In this study, the feature dependence analysis gives a greater understanding of the effect of various mixing parameters on the concrete compressive strength, which in turn



a. Instance 1 b. Instance 2

Fig. 8. Instances of local explanation based on SHAP.

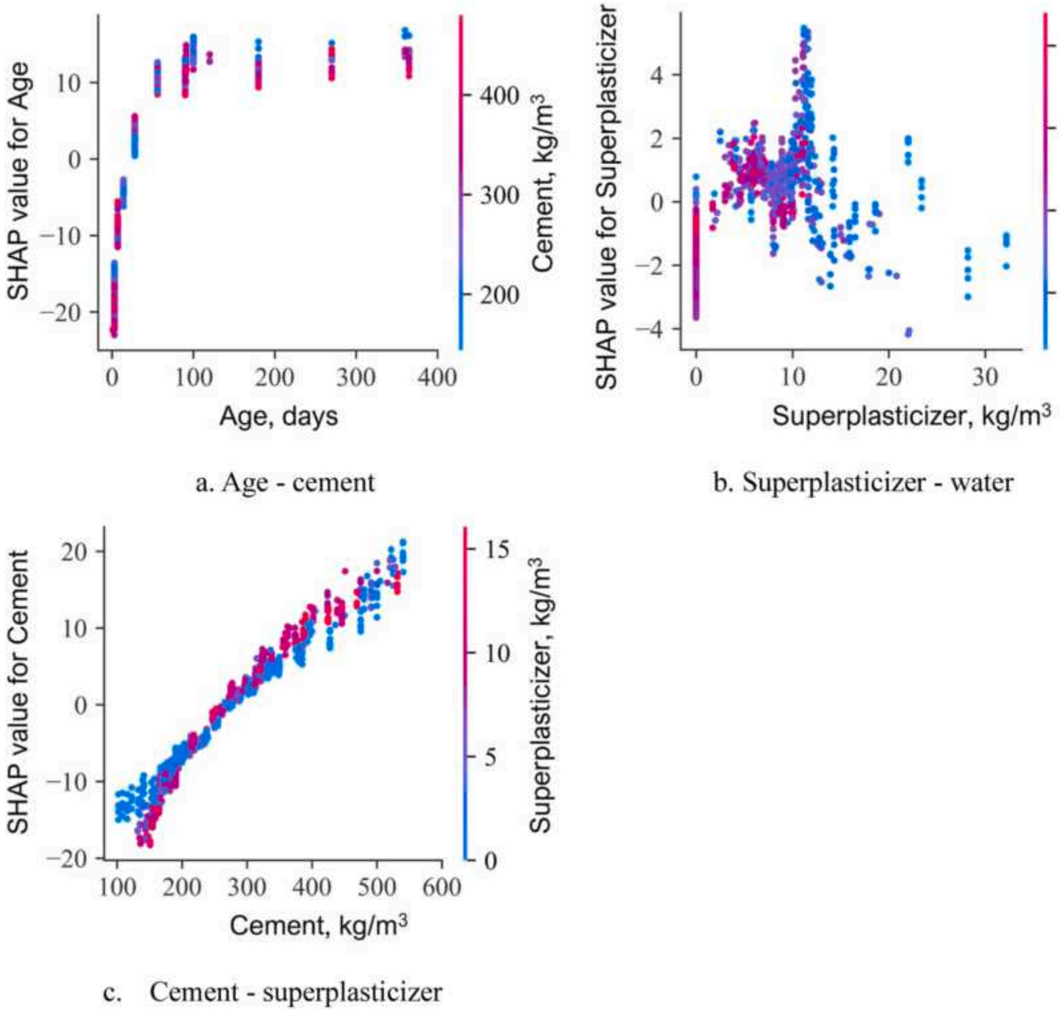


Fig. 9. Feature dependence plots.

provides guidance in the design of concrete mixes.

8. Conclusions

This study proposes an AutoML-SHAP (Automated Machine Learning - SHapley Additive exPlanations) strategy for predicting the compressive strength of concrete that is accurate, effective, and fully explainable. AutoML uses K-fold bagging and multilayer stacking to address the issues of model selection and hyperparameter tuning, automating the process of selecting the most suitable machine learning model and hyperparameters for a given dataset. This significantly reduces the time and effort required for these tasks. The proposed model's predictive performance was evaluated on a dataset containing 1030 sets of concrete compressive strength and compared with other typical ML models. Furthermore, the proposed AutoML model was made explainable by integrating with SHAP and the model outputs were interpreted in terms of global, local, and feature dependencies. The main findings of this study are summarized as follows.

1. AutoML automatically performs the processing of data splitting, hyperparameter tuning, model selection, and model stacking, while only the data engineering process needs to be manually processed. In terms of time effectiveness of modeling, the AutoML prediction model for concrete compressive strength is automatically established within 174 s of training time without manual adjustment of hyperparameters.
2. AutoML exhibits comparable predictive performance in the prediction of the compressive strength of concrete. It outperforms all the base ML models in the prediction of the test set with $R^2 = 0.96$, RMSE = 3.63, and MAE = 2.41. AutoML also exhibits a low dispersion of prediction errors and a high consistency between its predicted and actual values.

3. The global explanation of SHAP provides insight into the impact of each mixing parameter on the compressive strength of concrete. The local explanation visualizes the contribution of each feature in each prediction, making the concrete strength prediction process reliable and transparent. From the feature dependence analysis, the influence tendency of various mixing parameters on the concrete compressive strength can be obtained. The explainable mechanism of SHAP can assist in the concrete mixing design process.
4. The proposed AutoML-SHAP strategy complements the strengths of current state-of-the-art methods, accurately predicting the compressive strength of concrete and providing a fully interpretable model. Moreover, this method has strong generalizability and great potential for application in other fields of civil engineering.

In terms of limitations, this study only focuses on the prediction of compressive strength and does not consider other important properties of concrete, such as flexural strength and durability. Additionally, this study only considers a specific set of mixing parameters and does not take into account other potential factors that may affect concrete strength. Future research could consider incorporating more features and parameters to further improve the accuracy and explainability of the model. Furthermore, the proposed AutoML-SHAP model could be applied to other fields of civil engineering, such as predicting the strength of other construction materials or optimizing structural designs.

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.

Data Availability

Data will be made available on request.

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