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Towards Sustainable Construction Materials: A Comparative Study of Prediction Models for Green Concrete with Metakaolin

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Abstract: Cement-based materials are widely used in transportation, construction, national defense, and other fields, due to their excellent properties. High performance, low energy consumption, and environmental protection are essential directions for the sustainable development of cement-based materials. To alleviate the environmental pressure caused by carbon emissions in cement production, this paper studies cement-based materials containing metakaolin by a comparison of prediction models for the compressive strength. To more accurately evaluate the compressive strength of metakaolin cement-based materials, this paper compares the prediction effects of four models, namely, support vector machine (SVM), decision tree (DT), k-nearest neighbor (KNN), and random forest (RF), with hyperparameters optimized by the Firefly Algorithm (FA) to study the compressive strength of cement-based materials containing metakaolin. The results demonstrated that the RF model showed the optimized prediction effect considering the lowest RSME value and the highest R value among the hybrid models for predicting metakaolin cement-based materials' compressive strength. The importance test showed that the cement grade and the water-to-binder ratio greatly influence the compressive strength of cement-based materials with metakaolin compared to the other design parameters.

Keywords: metakaolin; green concrete; machine learning; compressive strength; hyperparameters

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1. Introduction

Cement-based materials refer to the materials with new properties obtained by combining cement with other materials [1–3]. Common cement base materials have concrete, mortar, and grouting materials [4–12]. Cement-based materials are widely used in construction, transportation, national defense, and other fields because of their advantages: high performance, convenient production, convenient construction, high compressive strength, good corrosion resistance, good durability, and so on [13–17]. In cement production, when $CaCO_3$, as cement raw material, decomposes into CO_2, the combustion of combustion materials also releases a certain amount of CO_2 [18]. Carbon emission has caused the greenhouse effect and brought a certain burden to the environment [4]. It is of great significance to improve the production of cement-based materials, effectively utilize resources, and alleviate the environmental load for promoting the sustainable development of cement-based materials [19]. Using mineral materials such as auxiliary gel materials to improve the performance of cement-based materials has become an important development direction in the manufacture of high-performance cement-based materials. The commonly used mineral materials are fly ash, silica fume, ore powder, metakaolin, and so on [20].

Mineral admixture can reduce the use of cement and reduce the cost and the carbon emission caused by cement production. In addition, mineral admixture can improve the performance and internal structure of cement-based materials and improve the strength and durability of cement-based materials [21,22]. Metakaolin is a kind of active mineral admixture formed by calcination of kaolin as raw material at high temperatures [23,24]. Metakaolin can be hydrated with cement to generate the corresponding cementing substance and improve cement-based materials' strength and corrosion resistance [25,26].

In recent years, there are many types of research on improving cement-based materials' performance by adding the appropriate amount of metakaolin into cement-based materials, mainly focusing on the compressive strength and durability of cement-based materials [27]. Metakaolin was used in the cement composite because it can significantly improve the properties of cement-based materials because of its pozzolanic activity, nucleation, and macroaggregates filling effect. Batis et al. studied the influence of metakaolin on the compressive strength and corrosion of cement mortar and found that the compressive strength of cement mortar could be improved by replacing cement with partial metakaolin. When the content of metakaolin is 10%, its contribution to the compressive strength of cement mortar is the largest. As a substitute for sand or cement, Metakaolin plays a positive role in improving the corrosion resistance of cement mortar [1,2]. Khater et al. studied the resistance of cement mortar with different amounts of metakaolin to magnesium chloride solution. The research results showed that the higher the metakaolin content within a certain range, the stronger the resistance of cement mortar to magnesium chloride solution [28]. Wang et al. evaluated various properties of metakaolin mixed concrete with the comprehensive hydration force durability model [4]. Kirsanova et al. studied the influence of metakaolin on the structural change of modified cement set to evaluate the influence of metakaolin on the phase composition of cement set. The results showed that the use of metakaolin promoted the composition of metastable calcium hydroaluminate and thus promoted the structure composition of cement set [29]. Kadri et al. studied the influence of metakaolin on hydration heat and compressive strength of mortar, and the results showed that adding a certain amount of metakaolin could bring mortar to a higher temperature. The contribution of metakaolin to mortar strength is mainly determined by packing effect, hydration acceleration of ordinary Portland cement, and pozzolans reaction of metakaolin [30]. Vu et al. studied the influence of metakaolin on the durability and compressive strength of cement mortar and concrete, and the research results showed that the replacement level of metakaolin for cement mortar or concrete was within 30%, and it had a positive effect on the compressive strength and durability of cement mortar and concrete [31]. Courard et al. found that metakaolin can inhibit chloride diffusion and sulfate erosion to a certain extent when the dosage of metakaolin is 5–20% of the mass of cement foundation by studying the durability of metakaolin on modified mortar [13].

Machine learning is an interdisciplinary subject involving many fields, such as probability theory, statistics, and algorithm complexity theory [32–38]. Machine learning mainly studies how to simulate and implement human learning behavior, acquire new skills, and constantly improve their skills [39,40]. The essence of machine learning is to process and analyze data in large quantities through the computer's powerful data processing and analysis ability [41–45]. In recent years, machine learning has been applied in many fields, such as finance, medicine, education, and architecture, due to its superior performance [35–37,46,47]. Many scholars at home and abroad have studied the application of machine learning in cement-based materials and made some progress [48–57]. Shamsabadi et al. studied the influence of waste marble powder (WMP) on the compressive strength of concrete by using the extreme gradient enhancement model (XGB) and artificial neural network model (ANN), and the results showed that the influence of WMP on the compressive strength of concrete was limited to 10–20% due to the inertia of WMP. Asteris et al. established an optimization model using a machine learning method to evaluate the impact of six input parameters on the compressive strength of metakaolin concrete: the specimen age, the metakaolin-to-glue ratio, the water–glue ratio, the superplastic fortifier ratio, and the thick–thin aggregate ratio [58]. Ahmad et al., based on Artificial Neural Network (ANN), Boosting, and AdaBoost machine learning, studied the prediction of compressive strength of high calcium fly ash base (GPC) based on Python coding. In addition, the comparison of the prediction performance of the two technologies showed that the ensemble ML method, AdaBoost, and Boosting method are better than the single machine learning technology in predicting the compressive strength of GPC [59]. Barnat-Hunek et al. proposed a new method based on image texture analysis and machine learning technology to evaluate Lightweight Cement composites with hydrophobic coatings modified by the durability of nanocellulose (LLC) materials [60]. Asteris et al. proposed to evaluate the applicability of cement mortar compressive strength based on traditional machine learning models, such as support vector machine, random forest, decision tree, and AdaBoost. The above machine learning methods have achieved good results in the performance evaluation of cement-based materials, proving that machine learning has a certain development prospect in the performance evaluation of cement-based materials.

Although some researchers used machine learning methods to evaluate the compressive strength of cement-based materials before, it should be pointed out that due to the characteristics and application of different machine learning models, their prediction effects for different application scenarios will be different to some extent [61,62]. However, in previous studies, few researchers have analyzed the influence of different machine learning methods on the compressive strength of cement-based materials with metakaolin. To more accurately study the influence of the cement grade, the water-to-binder ratio, the binder-to-sand ratio, the metakaolin-to-binder ratio, and the superplasticizer on the compressive strength of cement-based materials with metakaolin, this study will use FA to optimize the hyperparameters of SVM, DT, KNN, and RF. The prediction effect of these four models on the compressive strength of cement-based materials with metakaolin was compared, and the model with the best prediction effect was selected.

2. Methodology

2.1. Dataset Collection

A reliable and huge database is significant for predicting the compressive strength of cement-based materials containing metakaolin with machine learning models. In this study, data on the effect of the cement grade, the water-to-binder ratio, the binder-to-sand ratio, the metakaolin-to-binder ratio, and the superplasticizer on the compressive strength of cement-based materials with metakaolin were collected from published articles, and a reliable database containing 361 data sets was established. The influence of these five parameters on the compressive strength of cement-based materials with metakaolin has been confirmed in previous studies. Therefore, they were selected as the input variables in the present study; considering the fact that compressive strength has been regarded as one of the most important parameters to evaluate the performance of cement-based materials, it has been selected as the output variable. The database is randomly divided into the training set and testing set. The training set contains about 80% of the data in the database, whereas the testing set contains about 20% of the data. The frequency distribution histogram of the six variables is shown in Figure 1.

By comparing the predicted value and the actual value of the training set and the testing set of different machine learning models, the prediction effect of different machine learning models on the compressive strength of metakaolin cement-based materials was analyzed. The five machine learning models are introduced below.

Correlation analysis is an analysis method to verify the linear relationship between two variables through a correlation coefficient, which can analyze the correlation between two variables and the strength of the correlation. Before using the machine learning model to predict the compressive strength of cement-based materials containing metakaolin, it is necessary to analyze the correlation between the input variables. The correlation coefficient between the two variables is high positive or high negative, that is, there is a high positive or negative correlation between the two variables, which will affect the prediction effect of the machine learning model. The correlation analysis of the cement grade, the water-to-binder ratio, the binder-to-sand ratio, the metakaolin-to-binder ratio, and the superplasticizer is shown in Figure 2. As shown in Figure 2, the correlation between the same variables is 1, and that between different variables is 0.2–0.6. Although the correlation coefficients between the water-to-binder ratio and the superplasticizer, the water-to-binder ratio, the binder-to-sand ratio, the cement grade, and the binder-to-sand ratio are high, about 0.5, the correlation coefficients between them are all lower than 0.6, that is, these five input variables are independent of each other. Therefore, using these five variables as input variables to predict the compressive strength of cement-based materials with metakaolin will achieve good results.

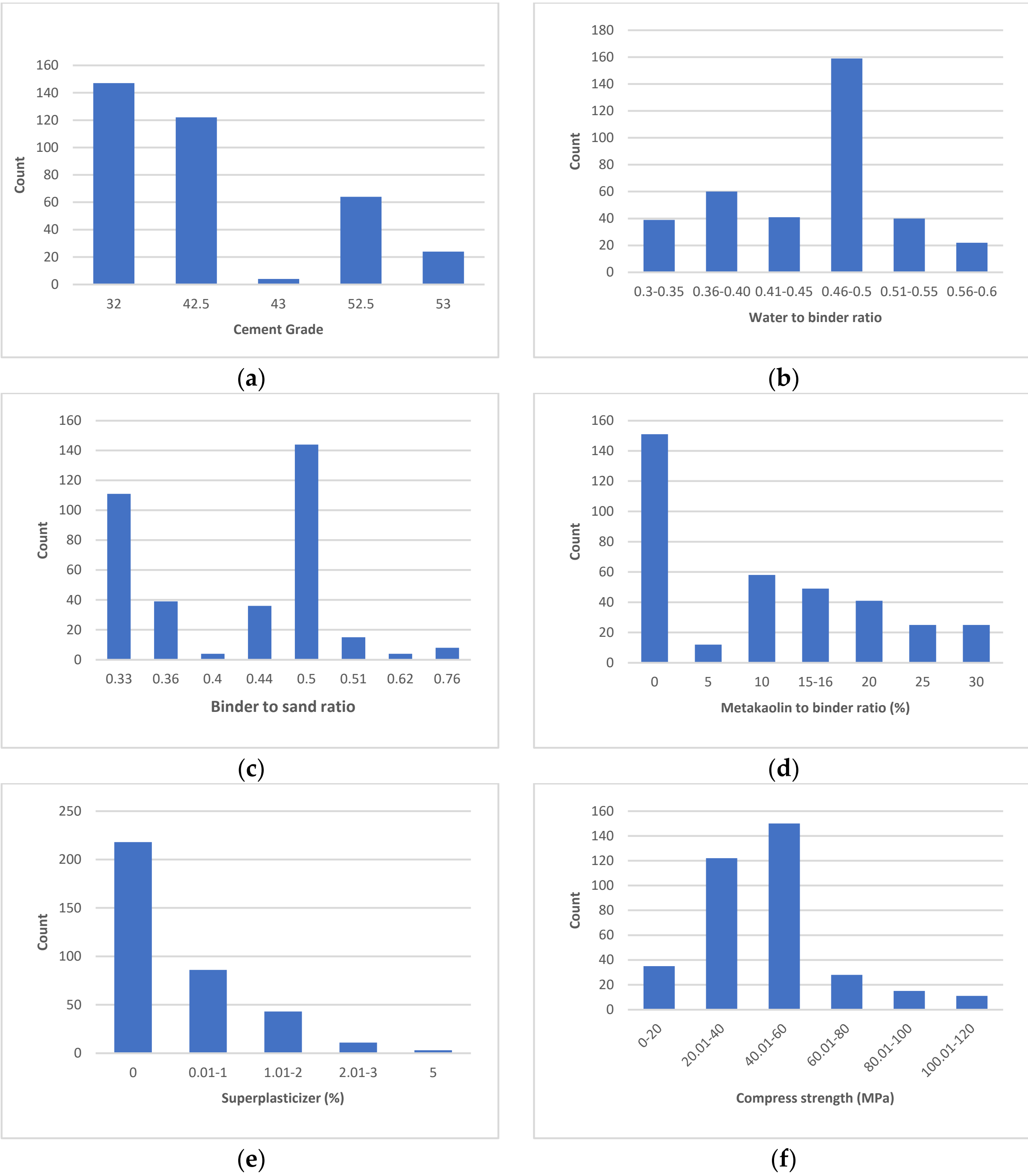


Figure 1. Frequency distribution histogram of variables. (**a**) Cement grade. (**b**) Water-to-binder ratio. (**c**) Binder-to-sand ratio. (**d**) Metakaolin-to-binder ratio. (**e**) Superplasticizer. (**f**) Compress strength.

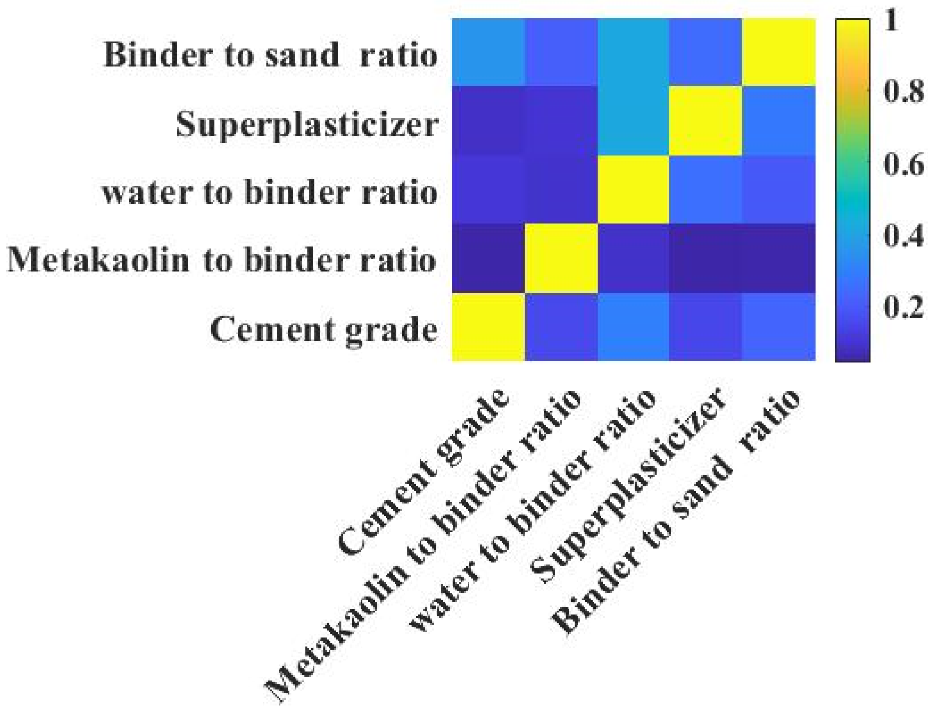


Figure 2. Correlation coefficients matrix diagram.

2.2. Applied Machine Learning Models

Five machine learning models, FA, SVM, DT, KNN, and RF, are used in this study, among which FA is used for hyperparameters tuning of the other four machine learning models. Four machine learning models including SVM, DT, KNN, and RF were used to predict the compressive strength of cement-based materials containing metakaolin with the cement grade, the water-to-binder ratio, and the binder-to-sand ratio, the metakaolin -to-binder ratio, and the superplasticizer as input variables.

FA is a random algorithm for global optimization problems based on firefly luminous behavior [63,64]. In the FA, it is assumed that all fireflies are hermaphroditic and are attracted to each other regardless of sex. FA is based on two key concepts: the intensity of the light emitted by the firefly and the degree of attraction between the two fireflies. The algorithm solves the optimization problem by simulating the living habits of fireflies attracted by light. The flow chart of FA can be found in Figure 3.

SVM is a method to classify data according to supervised learning. The decision boundary of the classification method is the maximum margin hyperplane of learning samples. SVM is suitable for small and medium-sized data samples, high latitude, and nonlinear classification problems [65]. High latitude means that SVM can efficiently deal with the classification of high-latitude feature space, which is of far-reaching significance in practical application. At the same time, although there are many training samples, SVM can only rely on limited samples for decision-making, so the computer only needs to store the limited samples used in decision-making, which saves the computer memory to a great extent [66]. DT is a predictive model in machine learning, representing the mapping between object attributes and object values. DT achieves the ability to predict target variables by input predictive variables by analyzing the relationship between input variables and target variables. A decision tree is similar to a flowchart in that each internal node is a test attribute and each branch is a test result. KNN is a data mining classification algorithm. Each sample in KNN can be represented by its nearest K neighboring values. This algorithm can classify every record in geometry. The idea of classification is that K samples are closest to each other in space, so the sample and the K samples belong to the same category. This method is a classification method to determine the classification of the samples to be classified by the category of one or several adjacent samples. RF is a common classification algorithm in machine learning. RF's basic idea is to establish a forest composed of many decision trees randomly, and there is no correlation between these decision trees. RF is mainly used to solve the classification problem. It uses multiple classification trees to classify data. In the process of classification, the algorithm obtains the importance of each variable classification by scoring the importance of each variable.

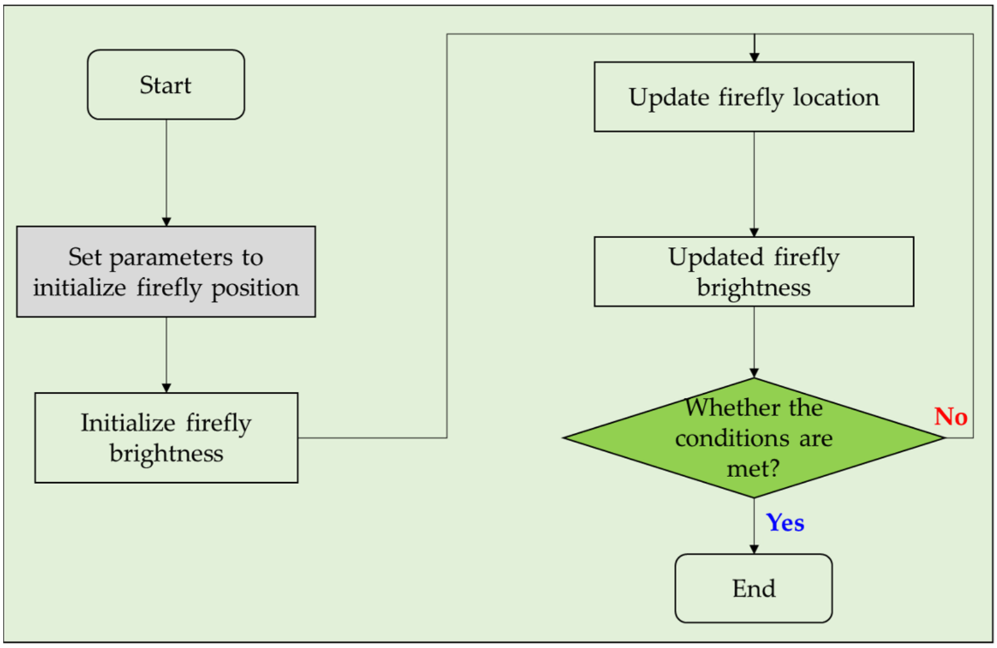


Figure 3. Flow chart of FA.

3. Results and Discussion

3.1. Hyperparameter Tuning

In this study, FA was used for hyperparameter tuning of SVM, DT, KNN, and RF models. The results of hyperparameter tuning are shown in Figure 4. As can be seen from Figure 4, with the increase in iteration times, RMSE values of these four models all decline sharply at first and then tend to be stable. The RMSE values of the SVM, DT, and RF models have similar rates of change, whereas the RMSE values of the KNN model are significantly different from those of the other three models, and its RMSE values are generally higher than those of the other three models, that is, FA has a poor tuning effect on this model. It can be seen from Figure 4 that after the hyperparameter tuning of SVM, DT, KNN, and RF by FA, the minimum RMSE values of SVM, DT, and RF models are all low, that is, the FA model has a better hyperparameters tuning effect on these three models. In this study, the prediction effects of four models, including SVM, DT, KNN, and RF on compressive strength of cement-based materials containing metakaolin after FA hyperparameter tuning were compared, and the model with the best prediction effect was selected.

The 10-fold cross-validation is a common test method to test the accuracy of the algorithm. This method needs to divide the data set into ten parts, selecting one of them as the testing data in turn and the remaining nine as the training data for training. The results of hyperparameter tuning for the above four models by 10-fold cross-validation are shown in Figure 5. Figure 5 shows that the minimum RSME of SVM, DT, and RF are all about 8, which are obtained at the fourth, ninth, and ninth iterations, respectively. The minimum RMSE value of KNN is 12, which is obtained at the sixth iteration. Therefore, after FA hyperparameter tuning, RSME values of SVM, DT, and RF models are lower, that is, the prediction effect of compressive strength of cement-based materials with metakaolin is better.

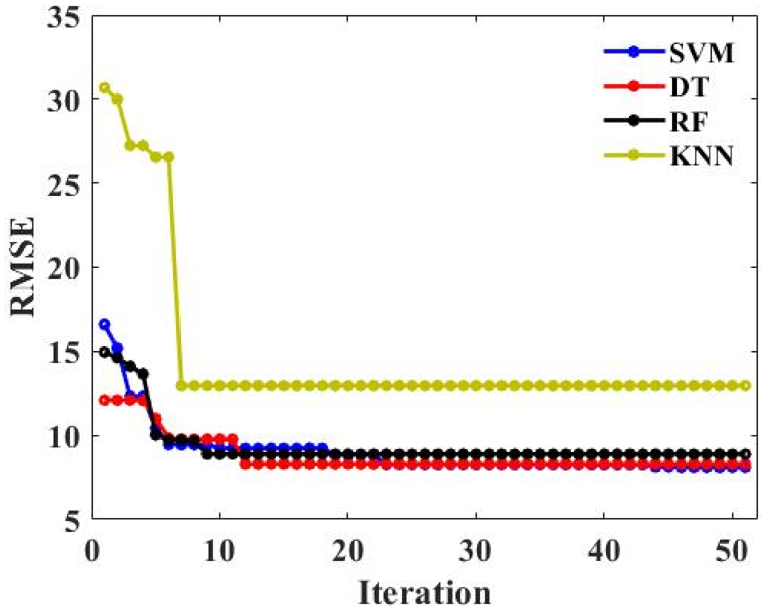


Figure 4. Root-mean-square error (RMSE) versus iterations.

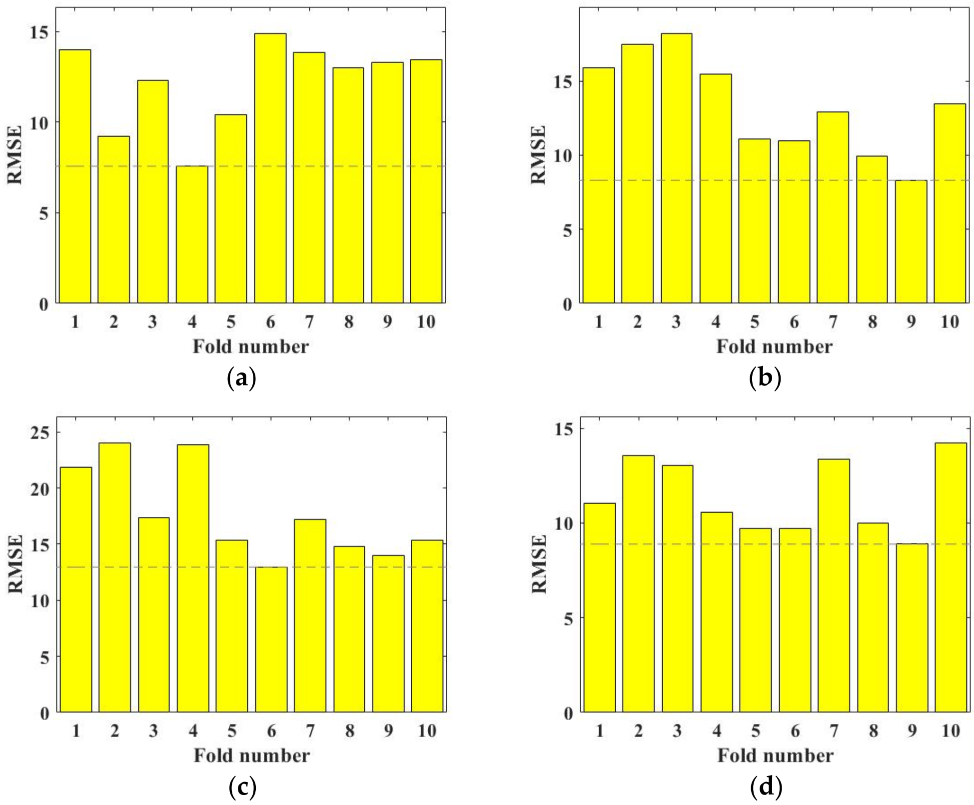
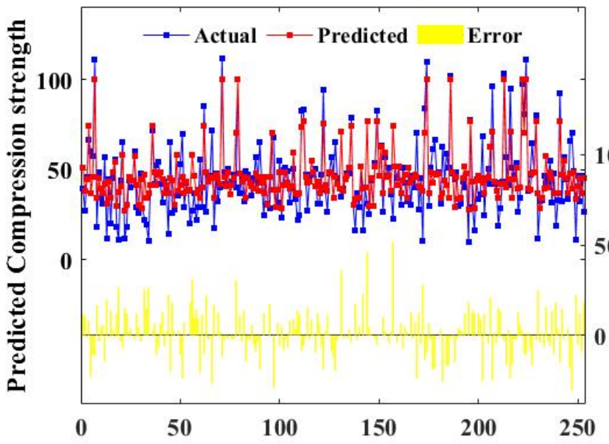


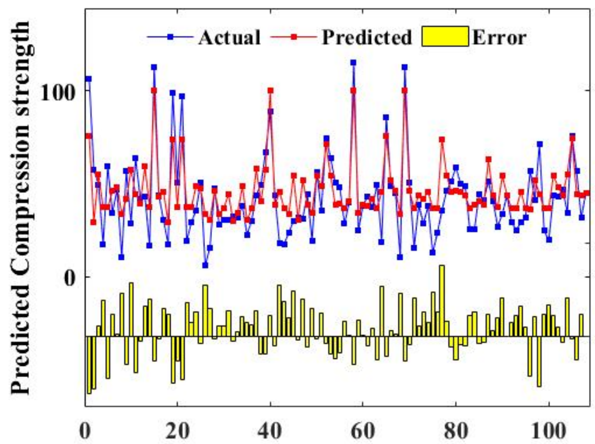
Figure 5. RMSE values of different folds. (**a**) RMSE values of different folds (SVM model). (**b**) RMSE values of different folds (DT model). (**c**) RMSE values of different folds (KNN model). (**d**) RMSE values of different folds (RF model).

3.2. Model Evaluation

In this study, the accuracy of the prediction of compressive strength of cement-based materials with metakaolin was evaluated by comparing the predicted values with the actual values of the training set and the testing set of SVM, DT, KNN, and RF. The comparison results between the predicted value and the actual value of the four models are shown in Figure 6, where the horizontal line represents the error between the predicted value and the actual value of the dataset. As shown from Figure 6, the predicted values and the actual values of SVM, DT, and RF are consistent, with only a few points with large errors, while there is a large error between the predicted values and the actual values of KNN.



(**a**)



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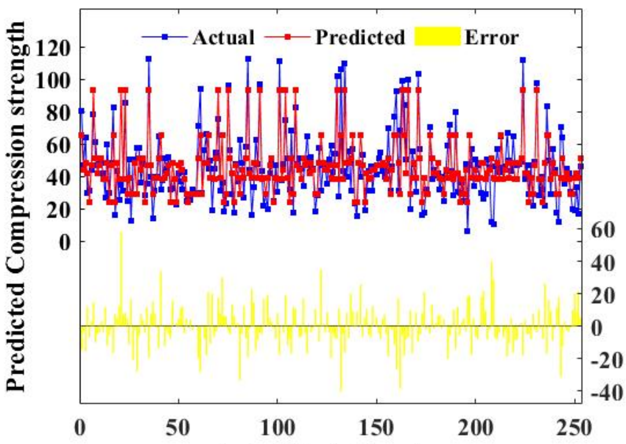

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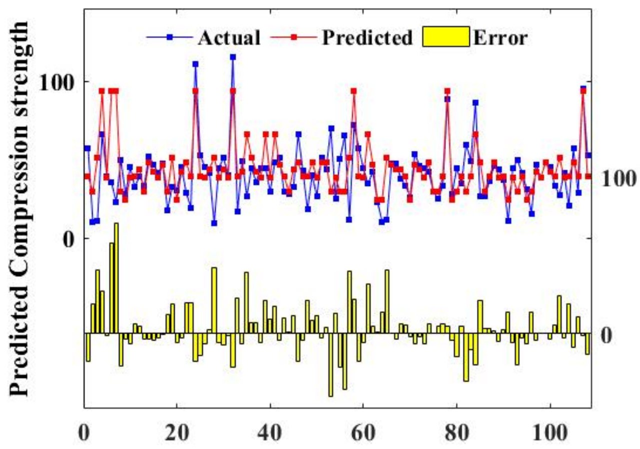

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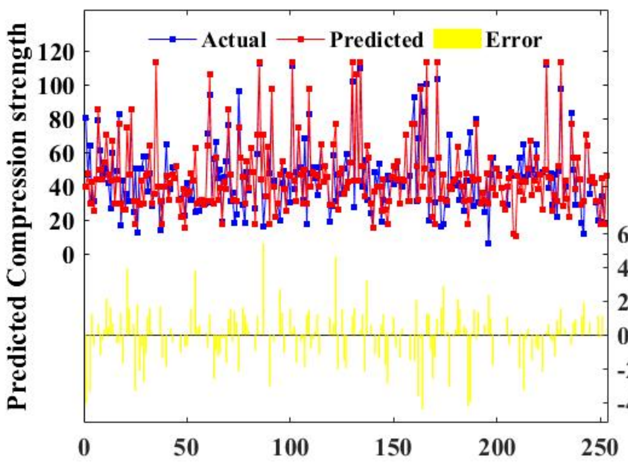

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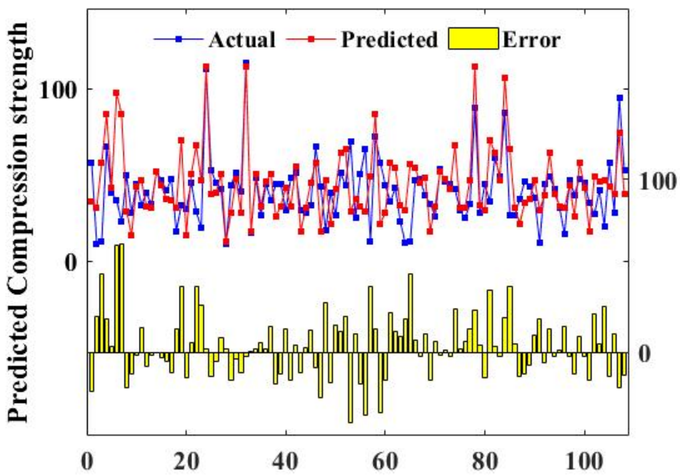
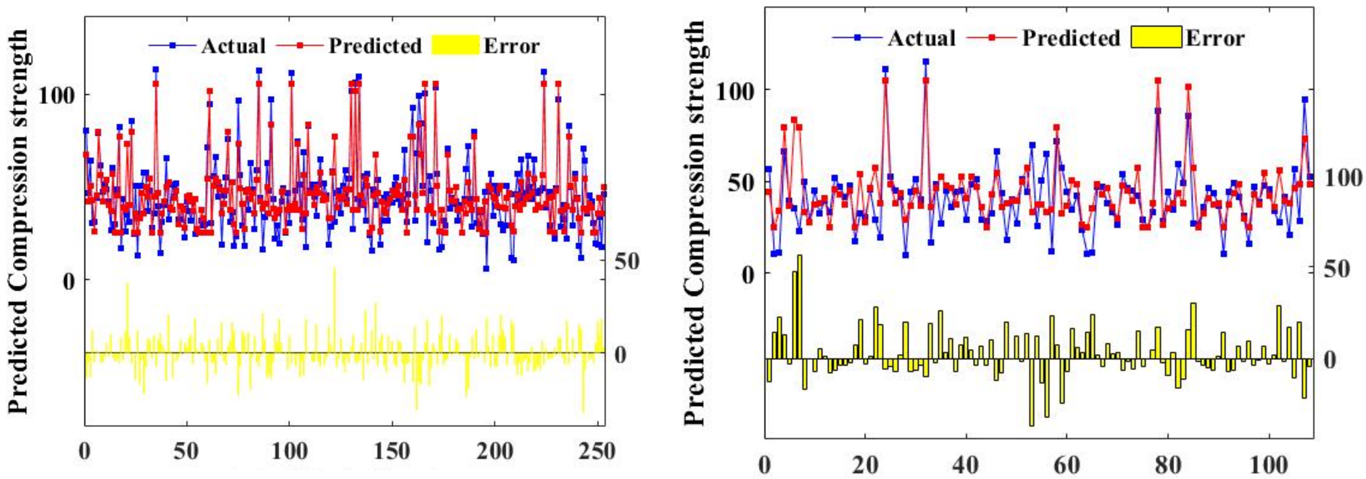


(**f**)

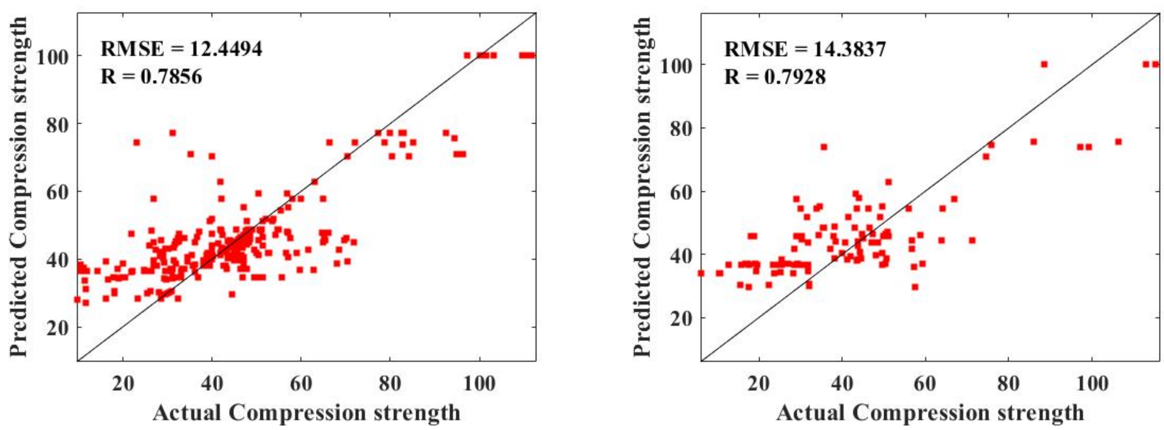
Figure 6. *Cont.*



(**g**) (**h**)

Figure 6. Comparison of the actual compressive strength and predicted compressive strength. (**a**) SVM model (training dataset). (**b**) SVM model (testing dataset). (**c**) DT model (training dataset). (**d**) DT model (testing dataset). (**e**) KNN model (training dataset). (**f**) KNN model (testing dataset). (**g**) RF model (training dataset). (**h**) RF model (testing dataset).

Figure 7 compares the predicted and actual values of the training set and the testing set of SVM, DT, KNN, and RF. It can be seen from Figure 7 that most of the predicted values of the training set and the testing set of SVM, DT, and RF models are concentrated in 20–60 MPa, most of the actual values are concentrated in 0–60 MPa, and a few of the predicted values and the actual values of the training set and the testing set are concentrated in 60–120 MPa. Most of the predicted values and the actual values of the training set and the testing set of the KNN model are concentrated in 0–60 MPa and a few are concentrated in 60–120 MPa. The RMSE values corresponding to the SVM, DT, KNN, and RF training sets are 12.4494, 12.942, 13.6014, and 10.4863, respectively, and the R values are 0.7856, 0.7933, 0.7924, and 0.8709, respectively. The RMSE values corresponding to the testing sets of these four models are 14.3837, 17.6971, 19.2549, and 14.2904, respectively, and the R values are 0.7928, 0.5246, 0.5492, and 0.696, respectively. Among the four models, RF has the lowest RMSE value and the highest R value on both the training set and the testing set, whereas KNN has the highest RMSE value and the lowest R value on both the training set and the testing set. That is, after the hyperparameters of SVM, DT, KNN, and RF models are adjusted by the FA model, RF has the best prediction effect on the compressive strength of cement-based materials with metakaolin, whereas KNN has the worst prediction effect.



(**a**) (**b**)

Figure 7. *Cont.*

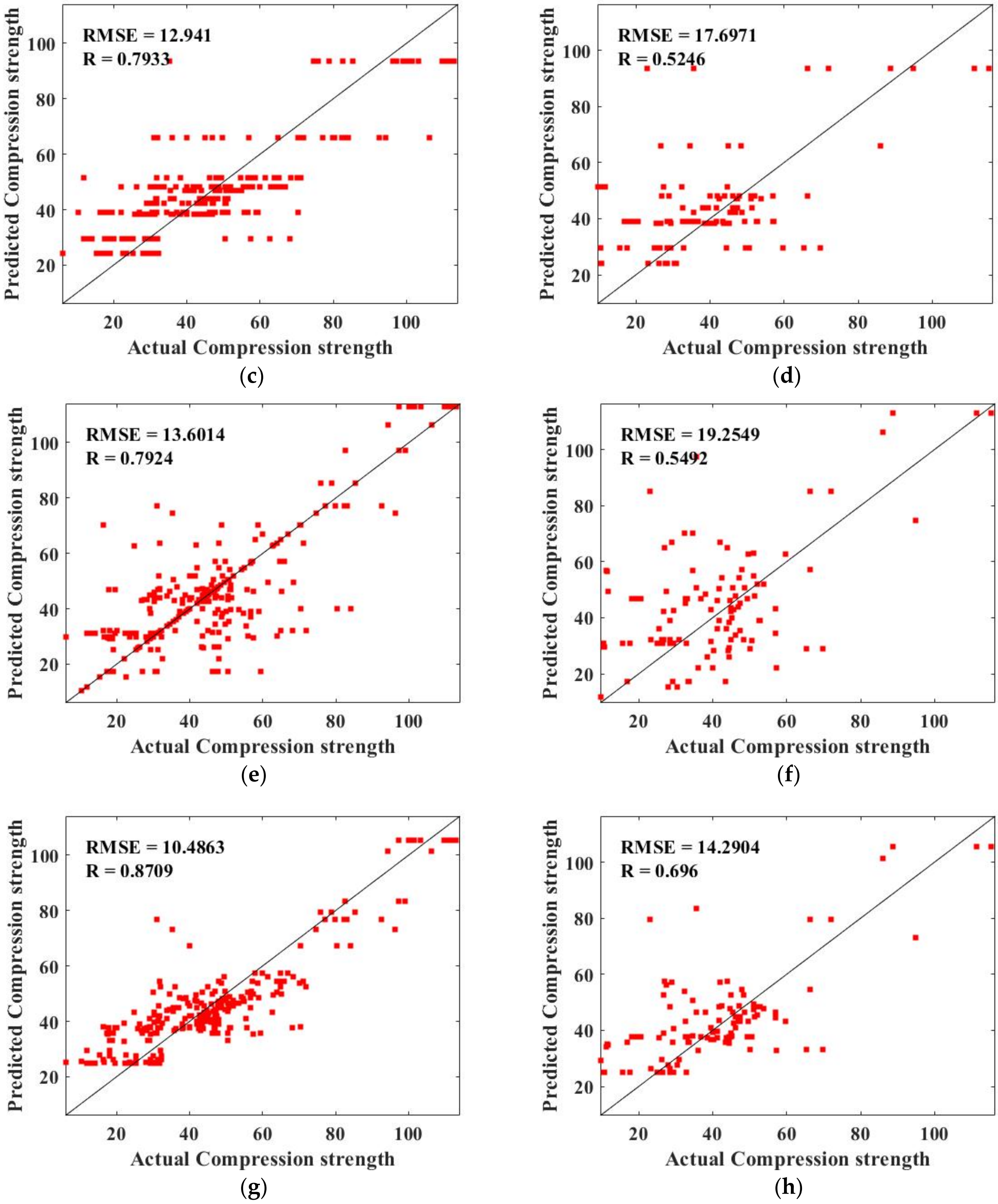


Figure 7. Comparison of the actual compressive strength and predicted compressive strength. (**a**) SVM model. (**b**) SVM model. (**c**) DT model. (**d**) DT model. (**e**) KNN model. (**f**) KNN model. (**g**) RF model. (**h**) RF model.

Figure 8 compares RMSE values and R values of SVM, DT, KNN, and RF with hyperparameter tuning by FA. It can be clearly seen from Figure 8 that after hyperparameter tuning by FA, RMSE values of these four models decrease one by one in the order of KNN, DT, SVM, and RF, while R values increase one by one. In other words, RF has the lowest RSME value and the highest R value among the four models, which confirms again that RF has the best prediction effect on the compressive strength of cement-based materials with metakaolin among the four models after FA hyperparameter tuning. Such prediction results can provide certain technical support in the production process of green concrete with Metakaolin in the future. However, it should be noted that the proposed model should be clarified before practical application, and the raw materials used should be consistent with the ones used to build the prediction model.

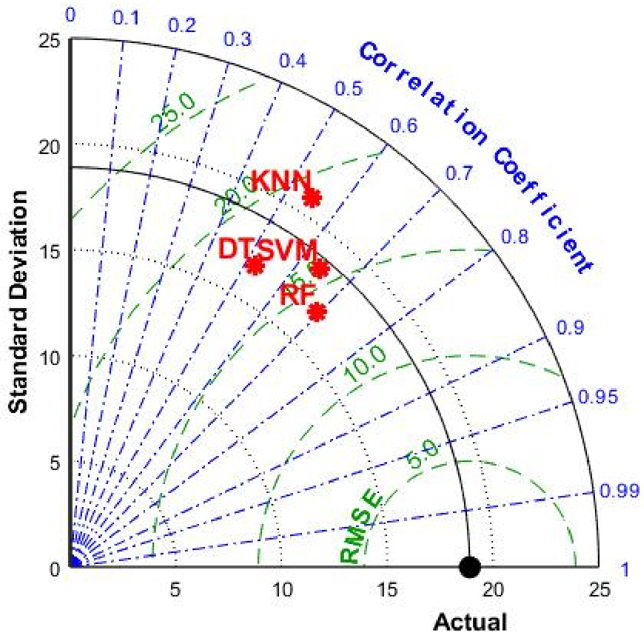


Figure 8. Comparison of RSME values and R values of different models.

3.3. Variable Importance Evaluation

Based on the analysis of the importance of the five input variables (the cement grade, the water-to-binder ratio, the binder-to-sand ratio, the metakaolin-to-binder ratio, and the superplasticizer) affecting the compressive strength of cement-based materials with metakaolin studied in this paper, we can understand the importance of these five variables to the compressive strength of cement-based materials with metakaolin and then provide some guidance for engineers to configure high-strength cement-based materials with metakaolin. Machine learning models can be used to predict the compressive strength of cement-based materials with metakaolin according to five input parameters: the cement grade, the water-to-binder ratio, the binder-to-sand ratio, the metakaolin-to-binder ratio, and the superplasticizer. Similarly, machine learning models can also be used to evaluate the importance of these five variables to the compressive strength of cement-based materials with metakaolin. According to the above analysis, RF is the best prediction model of SVM, DT, KNN, and RF after hyperparametric optimization with FA. Therefore, this paper will use the RF model to analyze the importance of the five input variables. It can be seen from Figure 9 that the importance of the cement grade, the water-to-binder ratio, the binder-to-sand ratio, the metakaolin-to-binder ratio, and the superplasticizer are all positive, that is, these five variables are directly proportional to the compressive strength of cement-based materials with metakaolin. Therefore, the compressive strength of cement-based materials with metakaolin can be improved by increasing any one of these five parameters. Among the five variables of the cement grade, the water-to-binder ratio, the binder-to-sand ratio, the metakaolin-to-binder ratio, and the superplasticizer, the importance scores of the cement grade and the water-to-binder ratio are the highest, which are 1.4400 and 1.4155, respectively, that is, these two parameters are the two most important variables affecting the compressive strength of cement-based materials with metakaolin. The importance score of the superplasticizer on the compressive strength of cement-based materials with metakaolin is 0.5981. Among the five input variables, it is the variable with the lowest importance score on the compressive strength of cement-based materials with metakaolin. Therefore, when configuring high-strength cement-based materials with metakaolin, engineers should focus on the impact of the cement grade and the water-to-binder ratio on the compressive strength of cement-based materials with metakaolin and do not need to focus too much on the dosage of the superplasticizer.

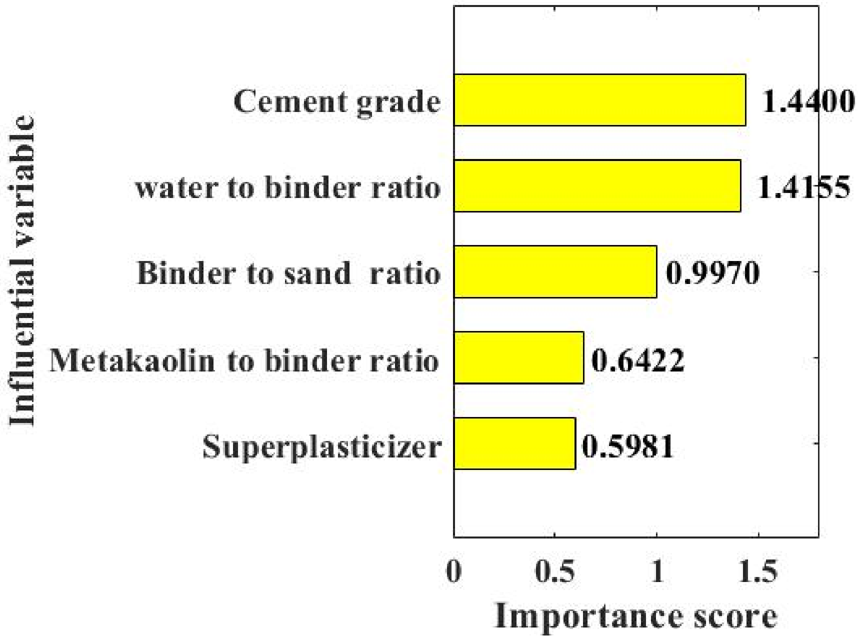


Figure 9. Variable importance of the compressive strength.

4. Conclusions

According to the published literature, this study established a database. The database takes the cement grade, the water-to-border ratio, the binder-to-sand ratio, the metakaolin-to-border ratio, and the superplasticizer as input variables, and the compressive strength of cement-based material with metakaolin as output variable. The data set in the database is randomly divided into the training set and the testing set. The training set contains about 80% of the data in the database, and the testing set contains about 20% of the data in the database. Based on using FA to tune the hyperparameters of SVM, DT, KNN, and RF, the author analyzed the model with the highest prediction accuracy of the compressive strength of cement-based materials with metakaolin by comparing the predicted values and the actual values of the training set and the testing set of these four models. The corresponding conclusions are as follows:

1. The FA model can achieve good results in the hyperparameter tuning of SVM, DT, and RF, whereas the FA model is relatively poor in the hyperparameter tuning of KNN. In other words, SVM, DT, and RF models can accurately predict the compressive strength of cement-based materials with metakaolin, of which the RF model has the best prediction effect, whereas the KNN model has the worst prediction effect.
2. The compressive strength of cement-based materials with metakaolin is directly proportional to the five variables of the cement grade, the water-to-binder ratio, the binder-to-sand ratio, the metakaolin-to-binder ratio, and the superplasticizer, that is, the compressive strength of cement-based materials with metakaolin increases with the increase of any one of these five variables. It decreases with the decrease of any one of these five variables.
3. The five variables of the importance of the compressive strength of cement-based material with metakaolin decrease one by one according to the order of the cement grade, the water-to-binder ratio, the binder-to-sand ratio, the metakaolin-to-binder ratio, and the superplasticizer. The cement grade and the water-to-binder ratio have a significant influence on the compressive strength of cement-based materials with

metakaolin. In contrast, the superplasticizer has less influence on the importance of the compressive strength of cement-based materials with metakaolin.

It should be noted that the predictive solutions may not be directly applied to the construction industry at present. This is because the 361 databases come from different studies, and there are significant differences regarding the raw materials in morphology characteristics, chemical composition, and other factors and the environmental parameters (such as the temperature). One goal of future research should be to establish a gene database of raw materials and take the genetic characteristics of raw materials (for example, morphology characteristics and chemical composition) as input variables to conduct in-depth data mining in the case of big data to establish reliable and effective prediction methods for actual production.

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