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Coal Spontaneous Combustion Temperature Prediction Based on an Interpretable Fusion Model

Yilong Xiao[#,*], Jidong Yao[#], Ruiyuan Su, Zecheng Zhu, Linxin Du, Xu Xia

College of Artificial Intelligence, North China University of Science and Technology, Tangshan, China

[#]These authors contributed equally

**Corresponding author*

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Abstract: This study proposes a stacking-SHAP method for predicting spontaneous combustion temperature, aiming to improve prediction accuracy and explain the decision-making process of the black-box model in order to develop targeted solutions for different spontaneous combustion fire scenarios. The method first performs data preprocessing and the construction of composite indices, then uses the Grey Wolf Optimization (GWO) algorithm for hyperparameter optimization of the base learners in the stacking fusion model, and finally predicts the test set. Experimental results show that the stacking model achieves a coefficient of determination (R^2) of 0.989, an average absolute error (EMA) of 6.003, a mean squared error (EMS) of 56.708, and an average logarithmic error (EMAP) of 6.34%. Comparison with the three base learners (GBDT, RF, and XGBoost) indicates that the stacking model outperforms them in terms of prediction accuracy and generalization ability. SHAP is used to interpret the stacking model, revealing the five most influential features on the prediction of spontaneous combustion temperature in the order of their impact: CO > O2/CO > CO2/O2 > CO2 > CO2/CO. Finally, ablation experiments confirm the accuracy of the SHAP interpretation method.

1. Introduction

Mine fire is one of the main disasters affecting the safety of coal mines [1], and spontaneous coal combustion is the main factor causing mine fires, and the prevention and control of spontaneous coal combustion has an important position in safeguarding the development of the national economy and guaranteeing the energy security [2], and the spontaneous combustion of coal will not only cause a large amount of coal resources to be wasted, but also produce a large amount of toxic gases, which will jeopardise the personal safety of workers in the underground mines [3], and mine safety has been highly valued by the central committee of the Party. Coal mine safety has been highly valued by the Party Central Committee, President has repeatedly emphasised that "production safety is a matter of people's well-being", and Premier Li Keqiang explicitly proposed in the third session of the 13th National People's Congress that "to ensure energy security, the first

priority is to promote the clean and efficient use of coal" [4]. Therefore, in the process of coal mining, it is necessary to carry out the monitoring of spontaneous coal combustion and ignition, and establish the monitoring system of spontaneous coal combustion and ignition.

2. Literature Review

The use of indicator gases is an important method for coal spontaneous combustion risk prediction, and many scholars have carried out related research. Zhai Xiaowei[5] used XK-VII large-scale coal spontaneous combustion experimental bench to simulate the natural ignition process of the 4-2 coal seam in Chaijiagou Mine, and analysed the parameters of spontaneous combustion characteristics, a single marker gas, and composite marker gases, deduced the range of the critical temperature of spontaneous combustion of coal seams and the dry cracking temperature, and the preferred indicator gases. An Jingyu[6] A study on the spontaneous combustion characteristics of No.2 and No.3 coal in a mine in Northwest China: the critical temperatures are 73.0°C and 72.1°C, CO is suitable for prediction at full temperature, and C2H4 and C2H6 are the preferred indicator gases after the dry cracking temperature. Jiang Heng [7] used grey correlation method to calculate the correlation degree values between 11 indicator gas concentrations or concentration ratios and coal temperatures, and the gas indicators were preferred based on the correlation degree values. H. Jiang [8] used grey correlation method to calculate the correlation degree values between 11 indicator gases' concentration or concentration ratio and coal temperature, and preferred the gas indicators based on the correlation degree values. Although the research on indicator gases has made great progress, the prediction accuracy needs to be improved.

With the emergence of machine learning, more scholars began to use machine learning algorithms to predict the temperature of spontaneous coal combustion. Deng Jun [9] et al. used particle swarm optimization algorithm (PSO) to optimize the support vector regression (SVR) parameters to establish a PSO-SVR model for coal spontaneous combustion temperature prediction, and the prediction accuracy was greatly improved. Zhou X [10] et al. proposed an XGBoost coal spontaneous combustion hierarchical early warning model combined with Bayesian optimization method, selected O2, CO, C2H4, etc. as indicator gases, and multiple models were compared to further validate the universality and stability of the BO-XGBoost model. Lei C [11] et al. proposed a coal spontaneous combustion prediction model based on the Random Forest method and based on the field data for testing, and also compared the neural network model, multivariate linear regression model, and the results showed that the random forest has better accuracy and prediction ability. Kong [12] et al. combined the logistic fitting model to fit the analysis of the indicator gas data with the curve of the coal temperature change, and established the coal spontaneous combustion grading early warning system based on the monitoring of the positive pressure beam pipe. And the CSC process was accurately classified into seven warning levels. Kong Biao [13] et al. proposed an improved whale optimisation algorithm combined with BP neural network (MSWOA-BP) for coal spontaneous combustion temperature prediction model. The validity of the model algorithm was verified based on the coal spontaneous combustion temperature rise experiments, and the prediction effect and performance of the particle swarm optimization (PSO-BP) model, the grey wolf optimization (GWO-BP) model, and the standard whale optimization (WOA-BP) model were further compared and analysed, and the results indicated that the MSWOA-BP prediction model had a higher prediction accuracy and stability. The introduction of machine learning has significantly improved the prediction accuracy, and the above study shows that machine learning has been widely used in the field of coal spontaneous combustion, however, at this stage of the research, the prediction is mainly carried out by using a separate model, which has a single prediction index, and it is difficult to explain the decision-making process of the

black-box model. For this reason, the stacking coal spontaneous combustion temperature prediction model is established by combining multi-source information fusion, and the SHAP interpretation method is used to explain the decision-making process of the model.

3. Methodology

In this study, the data were first cleaned, and conforming indicator construction was carried out based on the raw data to constitute the temperature prediction indicators. Subsequently, the data were preprocessed to remove outliers, fill in missing values, and standardize the data to eliminate the effect of magnitude. The processed data were then used for STACKING model training, and finally, the decision-making process of the STACKING model was interpreted using the SHAP method, as shown in Fig 1.

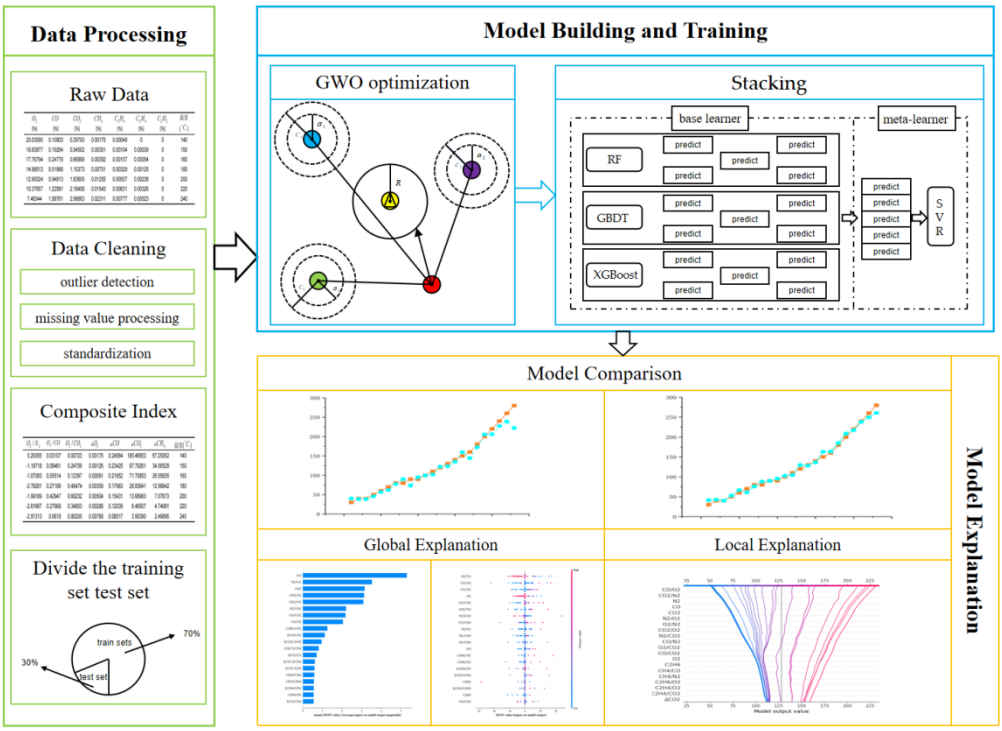

Figure 1 Technical Flow Chart

3.1 The Stacking Model

Stacking is a model fusion method [14], which involves an algorithm that integrates several different sub-models into a single framework. Its basic structure consists of two layers of algorithms: the first is the base learner, and the second is the meta-learner. For each base learner, training sets are constructed using a K-fold cross-validation method, which divides the dataset into K subsets. Each time, one subset is selected as the test set, while the remaining subsets serve as the training set, resulting in K predictions. The predictions from multiple base learners are then used as new features to train the meta-learner, which produces the final prediction. The method of model fusion can make the prediction better and reduce the risk of overfitting to a certain extent, this study adopts 5-fold cross-validation to construct a complete model using GBDT, Random Forest (RF), XGBoost as base learners and Support Vector Machine (SVR) as meta-learner, shown in Fig 2.

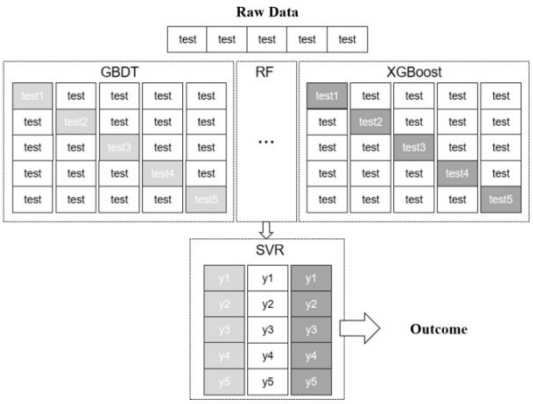

Fig. 2 Schematic diagram of stacking model

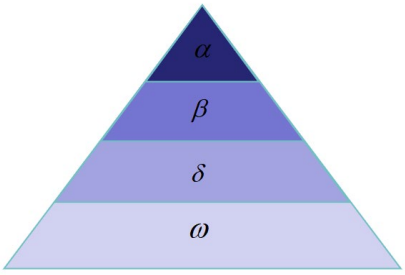

Fig. 3 Schematic diagram of the grey wolf hierarchy

3.2 GWO Optimisation Algorithm

GWO, developed by MIRJALILI and other scholars in 2014, is a meta-heuristic intelligent optimization algorithm based on the collaborative behaviour of grey wolf population [15]. The position of the grey wolf represents the possible solution of the optimization problem, and the prey represents the optimal solution of the problem. The GWO algorithm has the advantages of a simple structure, fewer parameters to be adjusted, and faster convergence. The algorithm grey wolf population is divided into four classes, and in the establishment of the mathematical model, the first four classes of grey wolves are defined as α, β, δ and ω, and the social classes are shown in Fig. 3.Grey wolf population hunting behaviour can be described by the following equation:

$$X(t+1) = X_P(t) - A \bullet D \tag{1}$$

$$D = \left| C \bullet X_P(t) - X(t) \right| \tag{2}$$

$$A = 2r_1 \bullet 2 \bullet (1 - \frac{t}{T}) - 2 \bullet (1 - \frac{t}{T}) \tag{3}$$

$$C = 2r_2 \tag{4}$$

Where $X(t)$ and $X(t+1)$ are the positions of the grey wolf at the t and $t+1$ iterations; $X_P(t)$ is the position of the prey, r_1 and r_2 are random variables in the interval [0,1], and T is the maximum number of iterations.

Since the location of the prey (optimal solution) is unknown, the model is built based on the property that α (potential optimal solution), β and δ have more knowledge about the location of

the prey, and the iterative process uses α , β and δ to guide the movement of ω to achieve global optimisation. The positions of α , β and δ are used to update the positions of all grey wolves using the following equations:

$$\begin{cases} X_1 = X_\alpha - A_1 \bullet D_\alpha \\ X_2 = X_\beta - A_2 \bullet D_\beta \\ X_3 = X_\delta - A_3 \bullet D_\delta \end{cases} \tag{5}$$

$$X(t+1) = \frac{(X_1 + X_2 + X_3)}{3} \tag{6}$$

Where X_α , X_β , X_δ and X denote the positions of α , β , δ and ω wolves in the n iteration respectively, and D_α , D_β and D_δ denote the distances between α , β , δ and ω wolves and preys respectively, the specific algorithm is shown in Fig 4.

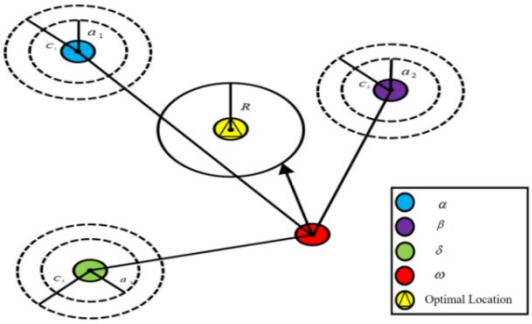

Fig. 4 Schematic Diagram of GWO Algorithm

3.3 SHAP Method

The SHAP method is a method for interpreting the prediction results of machine learning models [16]. It is based on the Shapley value in game theory and aims to assign importance values to each feature to help us understand the contribution of each feature to the model predictions. At the heart of the SHAP method is the Shapley value, which is a method for distributing the benefits in a cooperative game. Specifically, the Shapley value provides a fair allocation for each feature that takes into account the marginal contribution of that participant in different co-operative situations. In machine learning, the marginal contribution of a feature is the effect of adding a feature to the model output, taking into account other features. The Shapley value corresponding to feature i can be calculated using the following formula:

$$\varphi_i(f, x') = \sum_{S \subseteq F \setminus \{x_i'\}} \left[\frac{|S|!(M - |S| - 1)!}{M!} \times [f(S \cup x_i') - f(S)] \right] \tag{7}$$

$$f(S) = E[f(x) \mid x_s] \tag{8}$$

Where M is the total number of features; F is the set of all features; f is the original prediction model; x_i is the specific feature being interpreted; x_i' is the ith feature; S is the subset of features; φ_i is the Shapley value of the feature.

3.4 Assessment of Indicators

In order to evaluate the prediction accuracy of Stacking model, four evaluation indexes, namely, coefficient of determination R^2 , mean absolute error E_{MA} , mean square error E_{MS}, and mean logarithmic error E_{MAP} are used to reflect the prediction performance of the model, and compared with various single models to observe whether the prediction accuracy of the Stacking model has been improved.

4. Data Sources and Processing

4.1 Data Sources

The principle of spontaneous combustion of coal refers to the process of heating of coal by spontaneous reaction with oxygen in the air at room temperature and pressure. In this paper, we used the coal samples from each coal seam in Fan Ge Zhuang to carry out the procedure of warming experiments, to get the data of temperature and concentration of each gas, and to get the raw data as the following Table 1.

Table 1 Raw Data

O_2(%)	CO(%)	CO_2(%)	CH_4(%)	C_2H_6(%)	C_2H_4(%)	C_2H_2(%)	Temperature
20.03595	0.10803	0.29793	0.00175	0.00049	0	0	140
18.83877	0.19264	0.54502	0.00301	0.00104	0.00039	0	150
17.76794	0.24778	0.66899	0.00392	0.00157	0.00054	0	160
14.98513	0.51966	1.15373	0.00751	0.00329	0.00125	0	180
12.99324	0.94913	1.83605	0.01255	0.00557	0.00238	0	200
10.37657	1.22581	2.18458	0.01543	0.00631	0.00326	0	220
7.46344	1.88761	2.98663	0.02311	0.00777	0.00523	0	240

4.2 Data Pre-processing

Firstly, the outliers of the data are detected, and the adjacent values are replaced for the data where the gas concentration suddenly and abnormally increases or decreases, and some of the data do not conform to the real data intervals, and the existence of the total gas content is greater than 100 per cent, which does not conform to the real situation, and is eliminated. Vacant values are filled in using neighbouring data fitting, and after filling in, it is checked again whether it is an abnormal value, and if it is an abnormal value, it is eliminated. Composite indicators were constructed based on the processed data, and the constructed gas difference and inter-gas ratio data were introduced into the predictive indicators, as shown in Table 2 below:

Table 2 Composite Indicator Data

O_2/N_2	O_2/CO	O_2/CO_2	ΔO_2	ΔCO	ΔCO_2	ΔCH_4	Temperature
0.29355	0.03107	0.00723	0.00175	0.24564	185.46653	67.25052	140
-1.19718	0.08461	0.24709	0.00126	0.23425	97.79261	34.56528	150
-1.07083	0.05514	0.12397	0.00091	0.21852	71.70853	26.55935	160
-2.78281	0.27188	0.48474	0.00359	0.17983	28.83641	12.98842	180
-1.99189	0.42947	0.68232	0.00504	0.15431	13.68963	7.07673	200
-2.61667	0.27668	0.34853	0.00288	0.12039	8.46507	4.74991	220
-2.91313	0.6618	0.80205	0.00768	0.08517	3.95390	2.49895	240

In order to eliminate the effect of the dataset's magnitude on the predictive model, the processed data was normalised as follows:

$$x' = \frac{x - \mu}{\sigma} \tag{9}$$

Where x' is the normalised value; x is the value before normalisation; μ is the mean of the data; σ is the variance of the data.

5. Model Construction and Analysis of Results

5.1 Model Construction and Training Stacking-SHAP Model Construction

Step1:The processed data is divided into training set and test set in the ratio of 7:3, and the training set is divided into five subsets on average by using the five-fold cross-validation method, each time four of the subsets are input into the three base learners of RF, GBDT, and XGBoost for training, and prediction of the remaining one subset, and the training is carried out for five times, to get the prediction values of the three base learners on the training set.

Step2: The prediction results of the three base learners are used as new features, which are input into the meta-learner, the meta-learner is trained, and the prediction is performed in the test machine to constitute a complete stacking coal spontaneous combustion temperature prediction model.

Step3: The stacking model predictions are compared with the three base learners' predictions, and the models are comprehensively evaluated using evaluation metrics.

Step4: Interpret the stacking model using the SHAP method to derive the extent to which each metric influences the model's predicted results.

5.2 Parameter Optimisation

Multiple models are integrated in this model and a large number of parameters need to be set, so the GWO optimisation algorithm is used to optimise the parameters of each base learner to obtain the optimal parameters of the model using R^2 as the fitness function. The optimal parameters of each model after optimisation are shown in Table 3 below:

Table 3 Model Hyperparameter Optimisation Results

Modelling	Parameters	Optimal parameter values
GBDT	learning_rate	0.1
	max_depth	5
	min_samples_leaf	1
	min_samples_split	5
	n_estimators	100
RF	n_estimators	107
	max_features	0.8
	min_samples_split	2
	min_samples_leaf	1
	max_depth	10
XGBoost	n_estimators	174
	max_depth	1
	learning_rate	0.2
	min_child_weight	1.5
	subsample	1

5.2 Forecast Results and Comparative Analysis

The parameter optimised model was embedded in stacking model for training, and one of the coal seam sample data was selected for testing to get the final prediction results, and the results of comparing the prediction results of the four models with the real values are shown in Fig. 4:

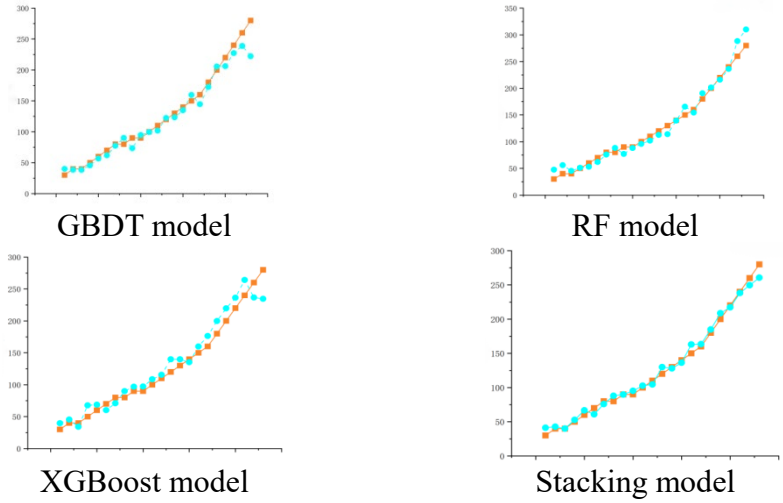

Fig. 4 Comparison of Predicted Results

Table 3 shows the comparison of the evaluation indexes of different models in the test set, where the value of R2 is in the range of [0, 1], and the closer it is to 1, the higher the accuracy of the model; EMA is the average of the absolute difference between the predicted value and the true value, which reflects the accuracy of the model's prediction; EMS is the average of the squared difference between the predicted and the true value, which emphasises the effect of larger errors; EMAP is the average of the ratio of the absolute error to the true value, which is expressed as a percentage, reflecting the relative error; and is the average of the ratio of the absolute error to the true value, expressed as a percentage, which reflects the relative error. The mean is the ratio of the absolute error to the true value, expressed as a percentage, reflecting the relative error.

Table 3 Results of Evaluation Indicators

Model	R^2	E_{MA}	E_{MS}	E_{MAP}
GBDT	0.955	9.987	231.230	8.21 per cent
RF	0.970	9.471	151.596	10.66 per cent
XGBoost	0.948	13.664	267.601	12.44 per cent
Stacking	0.989	6.003	56.708	6.34 per cent

Through model comparison, it can be seen that the stacking model is the most effective, with higher prediction accuracy and the strongest generalisation ability, its coefficient of determination R^2 is 0.989, the average absolute error E_{MA} is 6.003, the mean squared error E_{MS} is 56.708, and the average logarithmic error E_{MAP} is 6.34%, and all the four evaluation indexes are optimal, and the RF model is the most effective among the three base-learners, with the results of R^2 being 0.970, E_{MA} being 9.471, being 151.596 and being 10.66%. 9.471, E_{MS} is 151.596, E_{MAP} is 10.66%, the prediction performance of the four models is ranked as stacking > RF > GBDT > XGBoost. stacking model has a certain improvement in prediction effect compared to the three individual models, which is of great significance for the prediction of spontaneous combustion temperature of coal with high accuracy.

5.3 Interpretation of the model

In order to reveal the degree of contribution of each indicator in the model to the prediction results, the relationship between the input features in the stacking model and the prediction results is analysed using the SHAP method, and the global interpretation of some features is shown in Fig. 5, in which the horizontal coordinates of the feature importance plot represent the Shapley values of the features, and each point has to represent the degree of contribution of each feature in the sample, and the blue to red colour represents the degree of contribution is getting bigger and bigger. If a feature has a long-tailed distribution, it means that it will have a great influence on the prediction results; the bar chart shows the average Shapley value of the features, and the larger the average Shapley value, the greater the influence of the features on the prediction results in the whole sample. It can be seen that the five features with the greatest degree of influence on the prediction of coal spontaneous combustion temperature are in order $CO>O_2/CO>CO_2/O_2>CO_2>CO_2/CO$, the global interpretation of the features of the map demonstrates the dominant factors in the spontaneous combustion of coal fuming, which has an important significance for the implementation of specific measures [17].

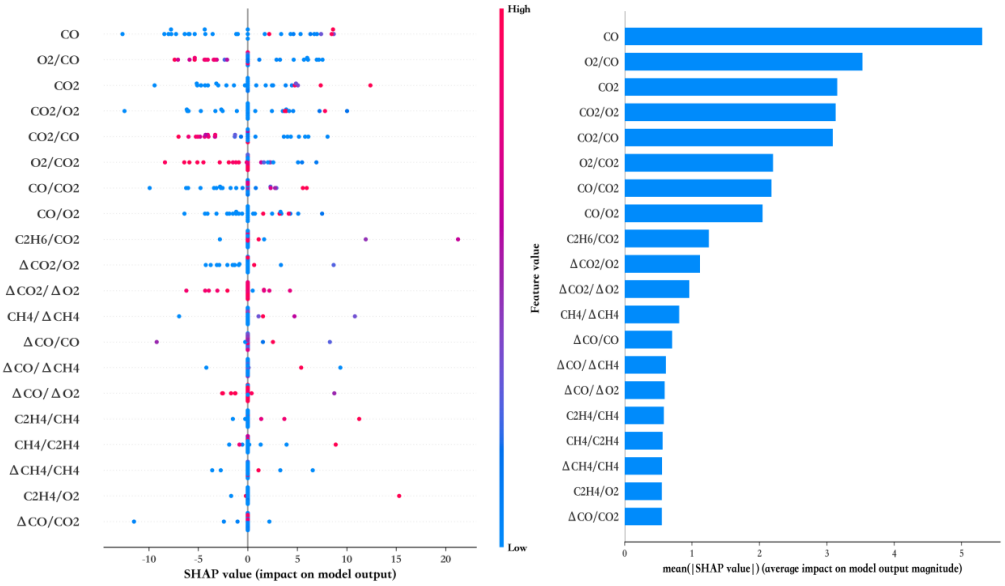

Figure 5 Global Interpretation Result Chart

Figure 6 shows the feature local interpretation plots for the sample data from two of the coal seams, the local interpretation plots provide insight into the individual sample predictions and help us to analyse how the model makes decisions based on the features. At the start of the decision plot there will be a baseline value representing the average prediction when the model does not have any input features, if a feature has a positive Shapley value this means that the feature is driving the predicted temperature up. Conversely, a negative Shapley value means that the feature is driving the predicted temperature down. The closer a feature is to the baseline value, the less impact it has on the prediction of the current sample. Conversely, the further away from the baseline value the feature is the more impact it has on the prediction.

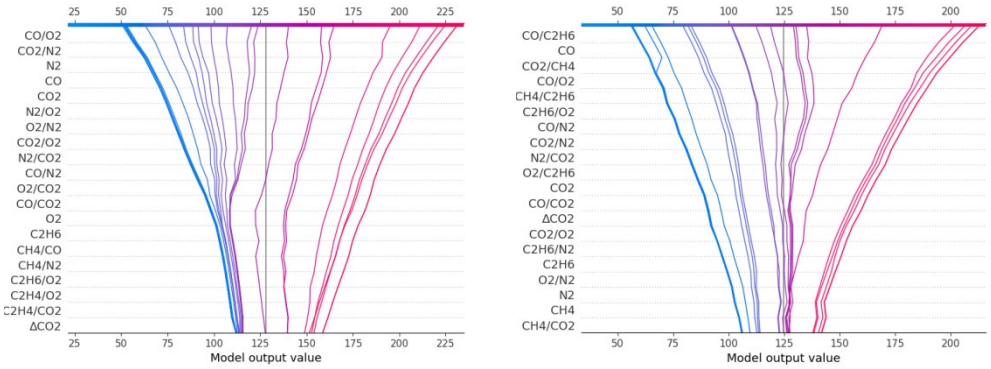

Fig. 6 Local Interpretation Result Map

5.4 Ablation Experiments

In order to study the effect of each feature on the model prediction more deeply and to verify the degree of feature contribution explained by the SHAP method, this study carries out ablation experiments, retrains the model by deleting certain input features with high Shapley values in the stacking model, and analyses the effect of the deleted features on the model prediction accuracy according to the prediction results [18]. In this study, five groups of experiments are set up to delete the five features with the highest mean values and analyse them in comparison with the model before deletion. In order to eliminate chance, one coal sample data is fixed as the test set for each group of experiments, and the rest of the coal samples are used as the training set.

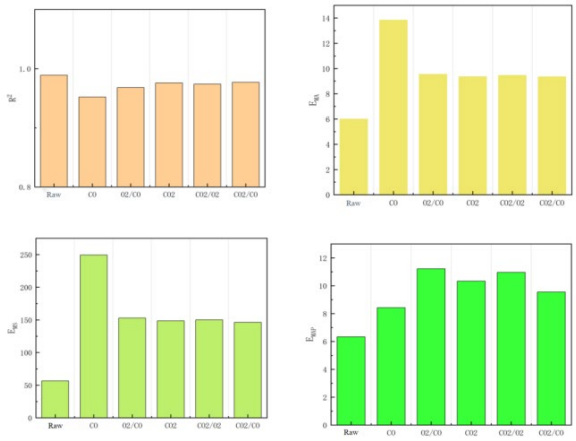

Fig. 7 Graph of Ablation Experiment Results

Figure 7 shows the prediction performance results of the stacking model ablation experiments, which can visualise the changes after the ablation experiments. It can be seen that among the five features selected for deletion, the one with the greatest impact on the model performance is *CO*, and after deleting the features, the model's R^2 decreases to 0.952, and the model's average absolute error E_{MA}, the mean squared error E_{MS} and the average pairwise error E_{MAP} increase; and the one with the least impact on the model performance is , and after deleting the features the model's decreases to 0.977. The smallest impact on the model performance is CO_2 / CO, and after removing the features, the model's R^2 decreases to 0.977. The input indexes influence the model's prediction performance in the order of $CO>O_2/CO>CO_2/O_2>CO_2>CO_2/CO$, which contributes to the same extent as the indexes interpreted by the SHAP method, which also verifies the accuracy of the SHAP's interpretation of the model's decision-making process and the indexes.

6. Conclusion

In order to further improve the accuracy of coal autogenous combustion temperature prediction and increase the interpretability of the black-box model, this paper proposes an interpretable model based on stacking-SHAP for coal autogenous combustion temperature prediction. The main work includes: (i) the construction of composite indicators on the data; (ii) the prediction of spontaneous coal combustion temperature by stacking integrated model; (iii) the optimisation of the GWO optimisation algorithm on the basis of the base learner in the stacking model to improve the accuracy of the model prediction; (iv) the use of the SHAP method to explain the decision-making process of stacking both globally and locally; and (v) the use of the ablation experiments to explore the effect of the indicators on the model prediction and to validate the accuracy of SHAP. Finally, the following conclusions are obtained:

(1) The stacking model is optimised by hyperparameters and finally the accuracy of temperature prediction in the test set is high its coefficient of determination R^2 is 0.989, mean absolute error E_{MA} is 6.003, mean square error E_{MS} is 56.708 and mean logarithmic error E_{MAP} is 6.34%.

(2) The stacking model shows a large improvement in prediction performance when compared to the three base learners GBDT, RF, and XGBoost.

(3) The SHAP method was used to interpret the stacking model, and the features that contributed more to the model decision were shown, of which the five features that contributed the most were, in order, $CO>O_2/CO>CO_2/O_2>CO_2>CO_2/CO$.

(4) The ablation experiment retrains the model by deleting the five metrics with the greatest degree of contribution, indicating that the degree of influence on the model's predictive performance is in the order of $CO>O_2/CO>CO_2/O_2>CO_2>CO_2/CO$, which is roughly the same as that interpreted by the SHAP method, verifying the accuracy of the SHAP method.

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