A Machine Learning-Based Prediction Method for Dynamic Fracture Toughness of Rocks

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Abstract

Dynamic fracture toughness of rock is a key parameter for evaluating the resistance of rock to crack propagation under dynamic loading, and is of great significance in engineering fields such as deep resource extraction and geological disaster prevention and mitigation. Traditional experimental methods face problems such as high cost and complex operation, whereas machine learning technology provides an efficient and low-cost solution for predicting dynamic fracture toughness. Based on experimental data from 210 groups of notched semi-circular bend rock specimens, this study selected density, elastic modulus, compressive strength, tensile strength, and loading rate as input variables, and employed six machine learning models, namely back propagation (BP) neural network, random forest (RF), support vector machine (SVM), extreme learning machine (ELM), long short-term memory network (LSTM), and convolutional neural network (CNN), to predict the dynamic fracture toughness of rock. Model performance was evaluated using the coefficient of determination (R2), relative mean absolute error (RMAE), relative mean bias error (RMBE), and relative root mean square error (RRMSE). The results show that the ELM and BP models perform best, with R2 values reaching 0.99 and 0.9865, respectively, demonstrating high prediction accuracy and good stability.

Full Text

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Abstract: Rock dynamic fracture toughness is a key parameter for evaluating the ability of rocks to resist crack propagation under dynamic loads, holding significant importance for engineering fields such as deep resource extraction and geological hazard prevention. Traditional experimental methods face problems such as high costs and complex operations, while machine learning technology provides an efficient and low-cost solution for predicting dynamic fracture toughness. Based on the data of 210 groups of rock specimens for notched semi-circular bending (NSCB) experiments, this paper selects density, elastic modulus, compressive strength, tensile strength, and loading rate as input variables, and uses six machine learning models—

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Rock fracture toughness is a key parameter characterizing the ability of rock materials to resist crack propagation under external loading, and it has important theoretical and practical significance for deep resource extraction, underground space development, and the prevention and control of geological hazards. The fracture behavior of rocks under static conditions has been widely studied[1-3]. Under dynamic loading conditions such as blasting, impact, or earthquakes, however, rock fracture behavior differs markedly from that under static loading, exhibiting complex changes in strain-rate effects, inertial effects, and energy-dissipation mechanisms[4]. Therefore, in-depth study of the testing methods, influencing factors, and micromechanical mechanisms of rock dynamic fracture toughness can not only improve the theory of rock dynamic fracture, but also provide a scientific basis for dynamic stability evaluation in engineering practice.

According to the crack loading mode and the direction of displacement, rock fracture toughness modes are mainly divided into three basic types—Mode I, Mode II, and Mode III—as well as combined modes (mixed modes)[5-7]. Because the tensile strength of rock is usually far lower than its shear strength, Mode I fracture is more common in rock engineering[8]. The International Society for Rock Mechanics (ISRM) has proposed various methods for determining the Mode I fracture toughness of rocks, including the chevron bend (CB) test[9], short rod (SR) test[9], cracked chevron notched Brazilian disc (CCNBD) test[10], and notched semi-circular bend (NSCB) test[11]. Under dynamic loading conditions, the NSCB test based on a split-Hopkinson pressure bar (SHPB) system has become the mainstream method for measuring Mode I dynamic fracture toughness, and ISRM has recommended it as a standard test method[12].

Based on this testing method, many scholars have carried out in-depth studies on the dynamic fracture toughness of different rock types. In research on rock-type specificity, scholars have analyzed the unique characteristics of dynamic fracture behavior arising from differences in the physical and mechanical properties of different lithologies. The study by PEI et al.[13] on reef limestone showed that dynamic fracture toughness has a linear relationship with density and exhibits a significant rate effect; the fracture toughness of saturated reef limestone is higher than that in the dry state, and differences in crystal morphology and arrangement cause cracks to propagate along grain boundaries, forming rough fracture surfaces. LIU et al.[14], through dynamic fracture tests on granite NSCB specimens and short core compression (SCC) specimens, combined with deep learning and scanning electron microscope (SEM) image analysis, found that the increasing proportion of shear-stress-dominated microscopic fracture morphologies with increasing loading rate is a key mechanism for the growth of dynamic fracture toughness, and that the sensitivity of Mode I fracture to loading rate is slightly higher than that of Mode II fracture. SONG et al.[15] investigated the dynamic fracture behavior of Beishan granite NSCB specimens and cracked chevron notched semi-circular bend (CC-NSCB) specimens, and found that the fracture toughness of both types of specimens increased with loading rate. Moreover, because stress concentration at the notch tip is more pronounced in CCNSCB specimens, their toughness values are generally higher; the evolution of the dynamic stress intensity factor in both specimens shows a three-stage pattern of "stable growth—sudden drop—secondary rise." In terms of loading-rate effects and microscopic mechanism analysis, scholars have explored the quantitative influence and internal mechanisms of loading rate on dynamic fracture toughness by controlling SHPB loading parameters. XING et al.[16] precisely measured the range of the dynamic Mode I fracture process zone at different loading rates and combined this with test results for crack-initiation toughness, finding that the range of the dynamic Mode I fracture process zone decreases as loading rate increases and that it has a significant influence on crack-initiation toughness. An increase in loading rate rapidly raises the degree of stress concentration at the crack tip, causing rapid crack propagation, so that the fracture process zone has insufficient time to develop fully; its range decreases, thereby affecting crack-initiation toughness. MAN et al.[17], combining macroscopic mechanical-property testing with microstructural analysis, showed that under dynamic conditions rock grains are crushed more severely and the energy-dissipation mechanisms are more complex. During dynamic loading, rocks instantaneously sustain high-energy impacts, and interactions among grains intensify, making grains more prone to crushing; at the same time, multiple energy-dissipation modes are generated, such as crack-propagation energy dissipation and frictional heat energy dissipation, making the energy-dissipation mechanism more complex. In studies on the regulation of environmental factors, scholars have combined practical engineering scenarios—such as deep high-temperature environments, freeze–thaw cycles in cold regions, and axial pre-stress in underground engineering—to extend the application boundaries of the SHPB-NSCB test. When studying the dynamic fracture toughness of granite under high-temperature environments, WU et al.[18] built a high-temperature SHPB test platform, heated granite specimens to different temperature ranges from 25 °C to 400 °C, and then conducted dynamic loading tests. The results indicated that, within this temperature range, fracture toughness increases linearly with loading rate, and that high temperature, by promoting crack closure and inhibiting microcrack propagation,

produce a strengthening effect. Under freeze–thaw cycling, Liu et al.[19] found that, after multiple freeze–thaw cycles, the dynamic fracture toughness of granite decreases significantly, with microcrack propagation and increased porosity being the main causes. Regarding the effect of axial prestress, Han et al.[20] showed that axial prestress reduces the dynamic fracture toughness of granite, and that the larger the prestress, the weaker the rate effect.

The above studies reveal the complex relationships between dynamic fracture toughness and loading rate, rock physical properties (density and porosity), environmental factors (temperature and saturation), and microstructure (crystal arrangement and crack path). However, traditional experimental methods still face challenges such as high cost, complicated operation, and large data scatter. In particular, under dynamic loading, it is difficult to precisely control stress-wave interference and inertial effects. Machine-learning technology therefore provides an efficient, low-cost alternative for this field. At present, most studies using machine learning to predict rock fracture toughness focus on static conditions. Chen Jinfan et al.[21] combined discrete-element simulation with machine learning to successfully predict the mode-I fracture toughness and crack-propagation patterns of rock specimens containing filled cracks, and developed a user-interface program to realize efficient batch prediction. Yang et al.[22] systematically evaluated the performance of multiple machine-learning models in the CCNBD and SCB tests recommended by ISRM, clarified the advantages and disadvantages of different models under different test conditions, and revealed through SHAP analysis the dominant role of tensile strength in predicting fracture toughness. However, no scholar has yet conducted machine-learning prediction of rock fracture toughness under dynamic conditions. Therefore, by training models with historical experimental data, this study enables machine learning to directly predict the dynamic fracture toughness of rocks under different loading rates on the basis of rock parameters. The trained models can be deployed as lightweight tools to realize real-time prediction and provide rapid support for rock-engineering applications.

1 Experimental Methods

1.1 Machine-Learning Models

The problems that machine-learning methods can solve can be broadly divided into data-regression prediction, data-classification prediction, and time-series prediction. In this study, predicting the dynamic fracture toughness of rocks under different loading rates through machine-learning models based on the mechanical parameters of rock specimens is a regression problem. The characteristics of the dataset are also crucial for selecting machine-learning models: dataset size, the types of data elements, and data structure are all key factors. In addition, the interpretability of machine-learning models also needs to be considered when selecting models. Considering the type of research problem, the characteristics of the dataset, and the interpretability of the machine-learning models, six machine-learning models—back-propagation neural network, random forest, support vector machine, extreme learning machine, long short-term memory network, and generalized convolutional neural network—were adopted to predict the dynamic fracture toughness K_{IC} of NSCB rock specimens under different loading rates.

1) A back-propagation (BP) neural network is a multilayer feedforward neural network[23] that adjusts weights and biases through error back propa-

gation to minimize prediction error. It has strong nonlinear fitting capability and is suitable for classification, regression, and pattern recognition.

2) A random forest (RF) is an ensemble algorithm composed of multiple decision trees[24]. It generates decision trees by randomly sampling data and features, and outputs the result through a voting or averaging mechanism. This method can reduce the risk of overfitting, is suitable for high-dimensional data, and can evaluate feature importance.

3) A support vector machine (SVM) is a supervised-learning algorithm[25] that seeks the optimal hyperplane to maximize the classification margin. For nonlinear data, kernel functions are used to map the data into a high-dimensional space for partitioning.

4) An extreme learning machine (ELM) is a fast learning algorithm for single-hidden-layer feedforward neural networks[26]. It randomly initializes the weights from the input layer to the hidden layer and uses least squares to calculate the output-layer weights. It has fast training speed and good generalization performance.

5) A long short-term memory (LSTM) network is a special recurrent neural network[27]. Through gate-control mechanisms (input gate, forget gate, and output gate) and cell states, it solves long-sequence dependence problems and is suitable for time-series prediction.

6) A convolutional neural network (CNN) is a feedforward neural network specifically designed to process grid-structured data[28]. It automatically extracts features through convolutional layers, pooling layers, and fully connected layers, reduces redundant information, and improves generalization ability.

1.2 Data Collection and Correlation Analysis

1.2.1 Data Collection

Based on published literature that measured the mode-I dynamic fracture toughness of NSCB rock specimens, only NSCB test data obtained using a split Hopkinson pressure bar (SHPB) system were included, and the test procedures conformed to the ISRM-recommended specifications for mode-I dynamic fracture-toughness testing[12]. This ensured consistency in loading method, specimen dimensions (diameter 50–100 mm, thickness 20–50 mm, and ratio of notch depth to radius 0.2–0.4), and data-calculation methods, thereby avoiding errors caused by differences in experimental principles. The 210 NSCB test samples obtained[14,16-18,20,29-38] cover a variety of typical engineering rocks, including granite, red sandstone, shale, marble, reef limestone, etc., so as to reflect the influence of different mineral compositions and structures on dynamic fracture behavior. The dynamic fracture toughness of the rock samples ranges from 0.29 to 9.23 $\mathrm{MPa \cdot m^{0.5}}$, and the loading-rate range is approximately 0 to 546 $\mathrm{MPa \cdot m^{0.5} \cdot s^{-1}}$, covering three typical dynamic loading conditions: low, medium, and high. All data came from SCI-indexed journals or domestic core journals, and the experimental procedures were all clearly

strictly followed the NSCB testing specifications recommended by the ISRM. Although the dataset has good diversity in terms of parameter types and rock types, it still has the following limitations: (1) slight differences in specimen geometry, machining accuracy, and boundary conditions among different studies may introduce certain systematic errors; (2) the data mainly come from laboratory-scale specimens, and the scale effects and geological heterogeneity in practical engineering are not fully represented.

The objective of this project is to predict the dynamic fracture toughness of specimens using machine-learning techniques; therefore, the rock dynamic fracture toughness K_{ICD} is the output variable. Based on the theoretical descriptions of rock dynamic fracture toughness in Refs. [39-41], one obtains

$$K_{\mathrm{ICD}}\left(E, \rho, \varepsilon_1'\right) = K_{\mathrm{ICQ}} K_{\mathrm{V}} \tag{1}$$

$$K_{\mathrm{V}} = \frac{1 + \left(v_l / v_m\right)^5}{\sqrt{1 - v_l / c_p}} \tag{2}$$

$$v_m = R c_{\mathrm{R}} \tag{3}$$

$$c_{\mathrm{R}} = \left[\frac{E}{2\rho(1+\gamma)}\right]^{1/2} \frac{0.87 + 1.12\gamma}{1+\gamma} \tag{4}$$

$$c_p = \left\{\frac{(1-\gamma)E}{(1+\gamma)(1-2\gamma)\rho}\right\}^{1/2} \tag{5}$$

$$v_l = \frac{\varepsilon_1' a m \left(\varepsilon_1 / \varepsilon_0\right)^m}{3\varepsilon_1 D_0^{1/3} \exp\left[\frac{\left(\varepsilon_1/\varepsilon_0\right)^m}{3}\right] \left\{\exp\left[\left(\varepsilon_1/\varepsilon_0\right)^m\right] - 1\right\}^{2/3}} \tag{6}$$

where K_{ICQ} is the quasi-static fracture toughness of the rock; K_{V} is the dynamic amplification factor of the rock; v_l (i.e., $\mathrm{d}l/\mathrm{d}t$) is the propagation velocity of internal mesoscopic cracks in the rock; v_m is the crack-branching velocity; c_{R} is the Rayleigh-wave velocity; c_p is the P-wave velocity; γ is Poisson' s ratio; ρ is the density; E is the elastic modulus; m, ε_0, and R are shape-related deformation parameters; D_0 is the initial damage; a is the initial crack length of the rock; ε_1 is the axial strain of the rock; and ε_1' is the loading rate applied to the rock. From Eqs. (1)-(6) and Refs. [39-41], it can be seen that the density ρ, elastic modulus E, and applied loading rate ε_1' of the rock are closely related to the dynamic fracture toughness. In addition, the compressive strength σ_c and tensile strength σ_t of the rock are also closely related to its dynamic fracture toughness, because they are jointly controlled by the internal microstructure, mineral composition, and defect distribution of the rock. The relationship between tensile strength and fracture toughness is the most direct: both characterize the ability of rock to resist tensile failure, and the macroscopic tensile strength is essentially determined by the fracture toughness of microscopic cracks. Compressive strength, by contrast, is indirectly associated with fracture toughness through the "compression-induced tensile cracking" mechanism; when rock is subjected to compression, the resistance to the growth of internal microcracks, namely the fracture toughness, directly affects the manifestation of macroscopic compressive strength. Therefore, in general, the higher the static strength indices of a given rock, the stronger its ability to resist dynamic crack propagation, that is, its dynamic fracture toughness. Accordingly, the density, elastic modulus, loading rate, compressive strength, and tensile strength of NSCB rock specimens are selected as input variables.

To obtain an intuitive understanding of the dataset, statistical analysis was performed on it. As shown in Fig. 1, a composite plot superimposing violin plots and box plots was used to simultaneously display the distribution density of the data and key statistical quantities. The central box plot represents the quartiles and median, while the outer envelope is the density-estimation curve, showing the density of the feature-data distribution; wider regions indicate that values are more concentrated, whereas narrower regions indicate that values are sparse.

Fig. 1. Violin plot reflecting the distribution characteristics of the dataset. Panels: (a) density; (b) elastic modulus; (c) compressive strength; (d) tensile strength; (e) loading rate; (f) dynamic fracture toughness.

1.2.2 Data Correlation Analysis

To analyze the correlations among the input variables, this study introduces the Pearson correlation coefficient [22]. The Pearson correlation coefficient is a statistical indicator used to measure the degree and direction of the linear relationship between two variables, and is expressed as

$$\rho_{x,y} = \frac{\sum(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum(x_i - \bar{x})^2 \sum(y_i - \bar{y})^2}} \tag{7}$$

where $\rho_{x,y}$ is the Pearson correlation coefficient between variables x and y (a positive value indicates a positive correlation, whereas a negative value indicates a negative correlation); x_i and y_i are the true values of variables x and y, respectively; and $\bar{x}$ and $\bar{y}$ are the mean values of variables x and y, respectively.

The Pearson correlation coefficient was used to analyze the sample data of the

NSCB rock specimens. The correlation coefficient can vary from −1.0 to 1.0, where −1.0 indicates a perfect negative correlation, 1.0 indicates a perfect positive correlation, and 0 indicates no correlation. As shown in Fig. 2, all five input variables of the NSCB rock specimens are positively correlated with K_{ICD}. The correlation between the input variable loading rate ε_1' and K_{ICD} is stronger than that of the other four input variables, reaching 0.93. In addition, relatively strong correlations are also found among ρ, E, σ_{c}, and σ_{t} in the NSCB specimens.

Fig. 2 Pearson correlation coefficient of the dataset

Fig. 2 Pearson correlation coefficient of the dataset

2 Model Result Analysis

2.1 Data Preprocessing

Selecting appropriate input variables is of great significance for improving the predictive capability of machine-learning models. Based on the analysis in Section 1.2.2, this study intends to use density, elastic modulus, compressive strength, tensile strength, and loading rate as input variables, and dynamic fracture toughness as the output variable. To accelerate model convergence, avoid numerical instability, and unify feature weights, the input and output variables in the dataset were normalized and scaled to the interval 0–1. Finally, all data were randomly shuffled to improve the generalization capability of the model, and the dataset was divided into a training set and a test set at a ratio of 8:2. The training set was used for hyperparameter tuning, training, and cross-validation, while the test set was used to evaluate the prediction performance of the trained model.

Through literature tracing $[14, 16-18, 20, 29-38]$, integrity checking and outlier detection were performed on the experimental data of 210 groups of NSCB rock specimens. It was found statistically that, when data for a single input variable of a certain type of rock (such as granite or sandstone in a specific region), for example elastic modulus E or tensile strength σ_{t}, were missing and could not be supplemented through literature tracing or verification by the authors, the "similar-rock, nearby-region data substitution method" was adopted. This method can reduce errors caused by cross-lithology and cross-regional data substitution. To avoid the influence of outliers on model prediction accuracy, a combination of box plots and violin plots (Fig. 1) was used to identify abnormal samples. Extreme values exceeding 1.5 times the interquartile range (IQR) beyond the upper and lower quartiles were regarded as outliers and removed.

2.2 Model Evaluation Metrics

To evaluate the prediction accuracy of different models and select the optimal model, this study introduced the coefficient of determination (R^2), mean bias error (R_{MBE}), mean absolute error (R_{MAE}), and root mean square error (R_{RMSE}).

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y}_i)^2} \tag{8}$$

$$R_{\text{MBE}} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i) \tag{9}$$

$$R_{\text{MAE}} = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i| \tag{10}$$

$$R_{\text{RMSE}} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2} \tag{11}$$

where y_i is the true value of the output variable; $\bar{y}$ is the mean value of the output variable; $\hat{y}$ is the predicted value of the output variable; and n is the number of experimental samples. R^2 measures the ability of the model to explain variations in the target variable (i.e., goodness of fit). The closer the value is to 1, the stronger the explanatory power of the model. R_{MBE} measures the systematic bias of the predicted values; a positive value indicates that the model overall underestimates, whereas a negative value indicates overestimation. R_{MAE} measures the mean absolute deviation between predicted and true values, with smaller values being better. R_{RMSE} measures the mean squared deviation between predicted and true values, is more sensitive to larger errors, and is also better when smaller.

2.3 Model Evaluation

MATLAB2023a was used to train six machine-learning models: BP, RF, SVM, ELM, LSTM, and CNN. The training and testing of all models used the same dataset. The performance of machine-learning models is closely related to the selection of hyperparameters. Table 1 lists the selected hyperparameters and their values for each model. Fig. 3 shows the training results of the six machine-learning models, while Fig. 4 shows the prediction results of these six trained models on the same test dataset. The closer the predicted values are to the 1:1 line, the more accurate the prediction. As shown in Fig. 4, all machine

All the machine-learning models showed strong performance on the test dataset. The test-set R^2 values for BP, RF, SVM, LSTM, ELM, and CNN were 0.9865, 0.9411, 0.9651, 0.9438, 0.99, and 0.9848, respectively.

Table 1 Selection and values of hyperparameters for the machine-learning models

Tab. 1 Selection and values of hyperparameters for the machine learning model

Machine-learning model	Hyperparameter	Value	Reason and explanation for selection
BP	Number of iterations	1 000	Ensures that the model has sufficient training cycles to converge while avoiding unnecessary computational overhead.
BP	Error threshold	1×10^{-6}	Sets a strict convergence criterion to ensure that model training reaches high accuracy.
BP	Learning rate	0.01	A relatively small learning rate is selected to ensure stability of the training process and to avoid oscillation near the optimal solution.
RF	Number of decision trees	100	Controls computational cost while ensuring model performance; an excessive number would lead to diminishing returns.

Machine-learning model	Hyperparameter	Value	Reason and explanation for selection
RF	Minimum number of leaves	5	Sets the minimum number of samples at which a node stops splitting, thereby controlling the depth of the decision tree and preventing overfitting.
SVM	Penalty factor	4.0	Balances the classification margin and classification errors; a larger penalty factor emphasizes penalties for classification errors and improves the fit to the training set.
SVM	Radial basis function parameter	0.8	Controls the width of the kernel function and affects the influence range of samples in the feature space; this value is determined through tuning to capture nonlinear relationships.

Machine-learning model	Hyperparameter	Value	Reason and explanation for selection
LSTM	Maximum number of iterations	1 500	RNN-type networks converge relatively slowly; the number of iterations is increased to ensure sufficient learning of sequence-dependence relationships.
LSTM	Initial learning rate	0.01	Uses a moderate learning rate to start training, ensuring the initial convergence speed.
LSTM	Learning-rate decay factor	0.1	Dynamically reduces the learning rate during training, helping the model converge stably to a local optimum in the later stage.

Machine-learning model	Hyperparameter	Value	Reason and explanation for selection
ELM	Number of hidden-layer nodes	50	Based on the number of input features and the sample size, a sufficient number of nodes is selected through trials to maintain strong nonlinear fitting capability while avoiding overfitting.
CNN	Maximum number of training epochs	1 200	Ensures that the convolutional layers and fully connected layers have enough update steps to extract effective features.
CNN	Initial learning rate	0.01	Similar to BP and LSTM, a stable and effective initial learning rate is selected.

Machine-learning model	Hyperparameter	Value	Reason and explanation for selection
CNN	Learning-rate decay factor	0.1	Dynamically reduces the learning rate during training, helping the model converge stably to a local optimum in the later stage.
CNN	Convolution-kernel size	3×1	Since the input features are one-dimensional vectors, a one-dimensional convolution kernel is used to perform local perception along the feature dimension, extracting local association patterns among features.

For the plots in Fig. 3, the vertical axis is the predicted value of K_{ICD}, and the horizontal axis is the true value of K_{ICD}.

- **(a) BP:** $R^2 = 0.9852$; $R_{\mathrm{MAE}} = 0.2341$; $R_{\mathrm{MBE}} = 0.0199$; $R_{\mathrm{RMSE}} = 0.3158$.
- **(b) RF:** $R^2 = 0.9319$; $R_{\mathrm{MAE}} = 0.3696$; $R_{\mathrm{MBE}} = -0.0102$; $R_{\mathrm{RMSE}} = 0.6884$.
- **(c) SVM:** $R^2 = 0.9765$; $R_{\mathrm{MAE}} = 0.3103$; $R_{\mathrm{MBE}} = -0.0282$; $R_{\mathrm{RMSE}} = 0.4219$.
- **(d) LSTM:** $R^2 = 0.9194$; $R_{\mathrm{MAE}} = 0.5858$; $R_{\mathrm{MBE}} = 0.0502$; $R_{\mathrm{RMSE}} =$

0.7565.

- **(e) ELM:** $R^2 = 0.9929$; $R_{\mathrm{MAE}} = 0.1517$; $R_{\mathrm{MBE}} = 0$; $R_{\mathrm{RMSE}} = 0.2116$.
- **(f) CNN:** $R^2 = 0.9858$; $R_{\mathrm{MAE}} = 0.2264$; $R_{\mathrm{MBE}} = -0.0083$; $R_{\mathrm{RMSE}} = 0.3009$.

Figure 3 Comparison between actual results and predicted results for the training datasets in various models

Fig. 3 Comparison between actual results and predicted results of training datasets in various models

In Fig. 4, the horizontal axis is the true value of K_{ICD}, and the vertical axis is the predicted value of K_{ICD}.

- (a) BP: $R^2 = 0.9865$, $R_{\mathrm{MAE}} = 0.266$, $R_{\mathrm{MBE}} = 0.028$, $R_{\mathrm{RMSE}} = 0.3459$.
- (b) RF: $R^2 = 0.9411$, $R_{\mathrm{MAE}} = 0.4353$, $R_{\mathrm{MBE}} = -0.0706$, $R_{\mathrm{RMSE}} = 0.6887$.
- (c) SVM: $R^2 = 0.9651$, $R_{\mathrm{MAE}} = 0.3466$, $R_{\mathrm{MBE}} = -0.0378$, $R_{\mathrm{RMSE}} = 0.4429$.
- (d) LSTM: $R^2 = 0.9438$, $R_{\mathrm{MAE}} = 0.4731$, $R_{\mathrm{MBE}} = 0.1321$, $R_{\mathrm{RMSE}} = 0.6474$.
- (e) ELM: $R^2 = 0.99$, $R_{\mathrm{MAE}} = 0.224$, $R_{\mathrm{MBE}} = 0.043$, $R_{\mathrm{RMSE}} = 0.3251$.
- (f) CNN: $R^2 = 0.9848$, $R_{\mathrm{MAE}} = 0.2644$, $R_{\mathrm{MBE}} = -0.0489$, $R_{\mathrm{RMSE}} = 0.3897$.

Fig. 4 Comparison between actual results and predicted results of testing datasets in various models

To select the optimal model for deployment as a lightweight tool, so as to replace complex NSCB tests in deep-resource extraction engineering, greatly reduce costs, and shorten the parameter acquisition cycle, Fig. 5 uses radial bar charts to compare the evaluation metrics of the six machine-learning models on the test set $(R^2, R_{\mathrm{MAE}}, R_{\mathrm{MBE}}, R_{\mathrm{RMSE}})$.

1) R^2 is used to measure the ability of a model to explain changes in the target variable. The closer its value is to 1, the higher the goodness of fit of the model. According to the test results, the ELM model has the highest R^2 (0.99), indicating that it has the strongest explanatory ability; next are CNN (0.9848) and BP (0.9865), which also perform extremely well. The R^2 values of RF and LSTM are relatively lower, at 0.9411 and 0.9438, respectively, but they still show good fitting ability.

2) R_{MAE} reflects the mean absolute deviation between predicted values and true values; the smaller the value, the better. ELM and CNN have the lowest R_{MAE}, at 0.224 and 0.2644, respectively, indicating that they have the highest prediction accuracy. BP and SVM follow closely, with R_{MAE}

values of 0.266 and 0.3466, respectively; RF and LSTM have slightly higher R_{MAE}, at 0.4353 and 0.4731, respectively.

3) R_{MBE} is used to evaluate the systematic bias of predicted values. The closer the value is to 0, the smaller the bias. A positive value indicates that the model overall underestimates the true value, whereas a negative value indicates overestimation. The test results show that BP, LSTM, and ELM underestimate the true values, whereas RF, SVM, and CNN overestimate the true values. Except for LSTM, the R_{MBE} values of the other models are small and close to 0.

4) R_{RMSE} is more sensitive to large errors; the smaller the value, the better the stability of the model. ELM has the lowest R_{RMSE} (0.3251), followed by BP (0.3459) and CNN (0.3897). The R_{RMSE} values of LSTM and RF are higher, at 0.6474 and 0.6887, respectively, indicating that their ability to predict extreme values is slightly weaker.

In Fig. 5, the four radial charts compare the following metrics for the six models:

- (a) R^2: RF 0.9411, BP 0.9865, CNN 0.9848, ELM 0.99, LSTM 0.9438, SVM 0.9651.
- (b) R_{MAE}: RF 0.4353, BP 0.266, CNN 0.2644, ELM 0.224, LSTM 0.4731, SVM 0.3466.
- (c) R_{MBE}: RF -0.0706, BP 0.028, CNN -0.0489, ELM 0.043, LSTM 0.1321, SVM -0.0378.
- (d) R_{RMSE}: RF 0.6887, BP 0.3459, CNN 0.3897, ELM 0.3251, LSTM 0.6474, SVM 0.4429.

Fig. 5 Comparison of performance metrics for six machine learning models on the test datasets

Because different evaluation metrics ($R^2, R_{\mathrm{MAE}}, R_{\mathrm{MBE}}, R_{\mathrm{RMSE}}$) emphasize different aspects of model performance, a single metric cannot fully reflect the overall performance of a model. Therefore, this study adopts a multi-index weighted scoring method to evaluate the six machine-learning models (BP, RF, SVM, ELM,

(LSTM, CNN) were compared systematically. The specific steps were as follows: first, the performance of the models under each evaluation metric was ranked, with the best performance receiving a score of 6.0. As the ranking decreased, the score decreased by 1.0. Specifically, the larger the value of R^2, the higher the score; the smaller the values of R_{MAE} and R_{RMSE}, the higher the score; and the closer the value of R_{MBE} was to 0, the higher the score. Then, the scores of each model under different evaluation metrics were accumulated to obtain the total score of the model. Based on the total model score, the comprehensive performance of the six machine-learning models could be evaluated. Although the learning process of machine-learning models can, to a certain extent, demonstrate the ability of a model to fit data, this study focuses more on the predictive performance of the models on the test dataset. The predictive-performance scores of the six machine-learning models on the test dataset are shown in Table 2. The ranking of these six machine-learning models from best to worst is ELM, BP, CNN, SVM, LSTM, and RF.

Table 2 Performance metric scores of different machine learning models

Tab. 2 Performance metric scores of different machine learning models

Machine learning model	R^2 score	R_{MAE} score	R_{MBE} score	R_{RMSE} score	Total score
BP	5	4	6	5	20
RF	1	2	2	1	6
SVM	3	3	5	3	14
LSTM	2	1	1	2	6
ELM	6	6	4	6	22
CNN	4	5	3	4	16

In summary, ELM and BP can predict the mode-I dynamic fracture toughness of NSCB rock specimens under different loading rates more effectively than the other four machine-learning models. This is because ELM and BP, as feedforward neural networks with strong nonlinear fitting capability, can effectively learn the complex constitutive response and energy-dissipation mechanisms of rocks under dynamic loading. In particular, in a high-dimensional feature space, both can better approximate the implicit relationships among the process-zone evolution, crack-growth rate, and macroscopic mechanical parameters during dynamic fracture, and therefore perform best on multiple evaluation metrics. However, the core advantage of CNN lies in processing grid-structured data (such as images). When it is used for predicting "one-dimensional physical parameters and dynamic fracture toughness," the one-dimensional parameters must be transformed into grid inputs, and this process may cause the loss of some physical information. SVM segments the data by searching for the optimal hyperplane. Even when a radial basis kernel function is used, its essence is still based on the assumption of "local linearization" ; however, rock dynamic fracture is a typical nonlinear process. RF outputs results through the voting mechanism of multiple decision trees, but its "binning" feature partitioning may simplify the continuous mechanical process of rock dynamic fracture. LSTM was originally designed to process time-series data (such as stock prices and temperature changes), and its gating mechanisms (input gate and forget gate) require reliance on "sequence information from preceding and subsequent time instants." In this study, however, all input features are static physical parameters; rock density, elastic modulus, and the like are intrinsic material properties, and the loading rate is a fixed condition in a single test. There is no "time-series correlation."

2.4 Analysis of Model Rationality and Interpretability

2.4.1 Rationality

In terms of coverage of model types, the six models encompass traditional neural networks, ensemble learning, kernel-function methods, fast-learning neural networks, time-series networks, and feature-automatic-extraction networks. They can comprehensively verify the applicability of different technical routes to the regression task of rock mechanical parameters. Among them, BP verifies the fitting ability of traditional neural networks for strongly nonlinear correlated parameters; ELM is suitable for engineering real-time prediction requirements; RF can evaluate feature importance to verify the key influence of loading rate; SVM handles complex implicit correlations among variables; and LSTM and CNN explore the application of time-series/grid feature-extraction logic to non-time-series data. From the perspective of data and cost matching, for the small- to medium-scale dataset of 210 groups of NSCB specimens, none of the six models requires extremely high computational resources. BP, ELM, and SVM can be trained and tuned quickly; although RF, CNN, and LSTM involve slightly larger computational loads, they can still be trained efficiently using MATLAB2023a, meeting engineering requirements of "low cost and easy deployment."In addition, this study did not select other advanced prediction models (such as XGBoost, LightGBM, Transformer, etc.). The main reasons are as follows: as advanced ensemble models, XGBoost and LightGBM require support from large samples to realize their advantages; with 210 groups of data, they are prone to excessive complexity and overfitting, and their accuracy may not necessarily be better than that of RF, while they increase the cost and difficulty of parameter tuning. Moreover, RF is already a representative decision-tree ensemble method, which avoids redundant comparison. Transformer relies on a self-attention mechanism, requires a large number of parameters and GPU support, and is difficult to deploy on conventional computers at engineering sites; furthermore, its training and parameter tuning are complex and the technical threshold is high. By contrast, the six selected models are simple to operate and easy to promote. The core objective of the study is to provide an "efficient and low-cost" prediction scheme for dynamic fracture toughness. The six models already cover the key technical routes and enable selection of the optimal model.

2.4.2 Interpretability

1) Random forest (RF): RF is based on the ensemble-learning mechanism of multiple decision trees. Its core advantage in interpretability is that it can directly output the relative importance ranking of each input parameter to the prediction results. This ranking essentially reflects the contribution differences of different rock physical and mechanical parameters in the

dynamic fracture process, and can directly correspond to rock-mechanics theory.

2) Support vector machine (SVM): The interpretability of SVM originates from its core principle of "searching for the optimal hyperplane to segment the data," especially when a radial basis function (RBF) kernel function is used.

when dealing with nonlinear problems, the model' s decision logic can be parsed through the geometric characteristics of the hyperplane. For regression-prediction tasks such as the dynamic fracture toughness of rocks, the regression hyperplane constructed by a support vector machine is essentially a mathematical expression of the mapping relationship "input-parameter combination–dynamic fracture toughness," while the distance (interval) from the sample point to the hyperplane directly reflects the reliability of the prediction result.

3) Back-propagation neural network (BP): The interpretability of a BP neural network must be analyzed from the two dimensions of "input-layer–hidden-layer weight distribution" and "gradient propagation from output to input." Although it is not as direct as a random forest, it can more deeply reveal the nonlinear coupling mechanism among parameters. The absolute values of the weights between neurons in the input layer and the hidden layer represent the contribution of the corresponding input parameters to feature extraction in the hidden layer: the larger the absolute weight value, the more critical the role of this parameter in constructing "dynamic-fracture-related features." This complements the feature importance of random forests: the former reflects the contribution of parameters to local features, while the latter embodies the global influence of parameters.

4) Extreme learning machine (ELM): Because an ELM has the characteristic of "randomly initializing the input-layer–hidden-layer weights and optimizing only the output-layer weights," its interpretability is slightly weaker than that of a BP neural network; however, the prediction logic can still be traced through hidden-layer node contribution analysis. Node contribution is calculated as "hidden-layer output value × output-layer weight," reflecting the role of each hidden-layer node in the final prediction, while the source of node contribution can be associated with specific input-parameter combinations.

5) Long short-term memory network (LSTM): The interpretability of an LSTM centers on the gate-control mechanism formed by the input gate, forget gate, and output gate; this mechanism endows the model with the ability to "remember–update"key information in sequential data. Although this study is not a typical time-series prediction problem, the parameter variation of "loading rate from low to high" can be regarded as a kind of "pseudo-sequence," and the logic by which the model captures the evolution law of dynamic fracture can be analyzed through changes in gate

activation values.

6) Convolutional neural network (CNN): The interpretability of a CNN must rely on the dual means of "local feature-extraction logic analysis" and "global contribution visualization." The core is to transform its implicit capture of nonlinear correlations between input parameters and dynamic fracture toughness into an explicit mechanism that can respond to rock-mechanics theory. The convolutional layers use convolution kernels of preset sizes to perform sliding-window feature extraction on the input parameters. The weight distribution of the convolution kernels directly determines the physical attributes of the captured local features (for example, if the weight of a certain convolution kernel for elastic modulus is the highest, then it focuses on "local features dominated by elastic modulus," reflecting the influence of the deformation-energy storage capacity of the rock on crack propagation), directly eliminating concerns that "feature extraction in deep models lacks physical meaning."

3 Conclusions

Based on existing experimental and theoretical studies on the dynamic fracture toughness of rocks, this study summarized five key parameters affecting rock dynamic fracture toughness and collected 210 groups of NSCB rock-specimen experimental data. The dataset was divided into a training set and a test set at a ratio of 8:2, and six different machine-learning models were trained and tested accordingly. The performance of the six machine-learning models was systematically compared, and the main conclusions are as follows.

1) Data correlation analysis shows that the Pearson correlation coefficient between loading rate and dynamic fracture toughness reaches 0.93, indicating that loading rate is a key factor affecting dynamic fracture toughness. Rock density, elastic modulus, compressive strength, and tensile strength are also positively correlated with dynamic fracture toughness and can serve as effective input parameters.

2) Among the six machine-learning models, the extreme learning machine (ELM) has the best overall performance, with R^2 on the test set of 0.99, R_{MAE} of 0.224, R_{MBE} of 0.043, and R_{RMSE} of 0.3251. Its fast learning characteristics and strong generalization ability make it suitable for real-time prediction of dynamic fracture toughness. The back-propagation neural network (BP) performs second best, with R^2 of 0.9865 and relatively good stability.

3) Machine-learning models can effectively avoid error sources such as stress-wave interference and inertial effects in traditional tests. Models trained in advance can predict dynamic fracture toughness under different loading conditions in real time. Among them, the ELM and BP models, owing to their high accuracy and stability, can be directly deployed as lightweight tools to provide rapid reference for blasting design and

hydraulic-fracturing parameter optimization in deep-resource extraction, thereby reducing engineering costs.

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