Deep learning-aided prediction of peak shear strength of rock fractures

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ABSTRACT: A robust estimation of peak shear strength of rock fractures in engineering practice is significant, but the three-dimensional (3D) surface characteristics of fractures have not been comprehensively quantified in the existing models. In this study, a deep learning-aided prediction method is proposed to estimate peak shear strength of rock fractures by considering the 3D surface roughness characteristics. The dataset is generated by numerical simulations after experimentally calibrated, and contains four features (normal stress, rock mechanical properties, relative fracture elevation). The deep learning model (FracSNet) assisted by data augmentation and fine-tuning is developed to provide reliable peak shear strength prediction of artificially-split fractures. The prediction ability is validated utilizing experimental data, and the results demonstrate that FracSNet can provide reliable prediction. The deep learning model of rock fractures has great a potential in engineering application with limited access to experimental data.

Keywords: Peak shear strength, Rock fractures, Particle-based discrete element method, Deep learning.

1 INRODUCTION

Peak shear strength (PSS) of rock fractures is a significant but challenging design parameter in rock engineering, affected by numerous factors and hard to precisely determine. A huge number of theoretical and empirical criteria have been proposed since the 1960s, including those considering two-dimensional (2D) geometric features of fracture profiles (e.g. Patton 1966, Ladanyi & Archambault 1969 and Barton & Choubey 1977) or others considering 3D features of fracture surfaces (e.g. Grasselli & Egger 2003, Ma et al. 2020 and Ding & Li 2021). In recent studies (Wu et al. 2019, Huang et al. 2021 and Fathipour-Azar 2022), machine learning (ML) approaches were used to create data-driven PSS criteria.

However, quantification of the fracture surface is complicated, single roughness parameters may cause information loss while several parameters may cause fitting problem. The existing data-driven criteria essentially only replaced the artificial equation fitting with ML model training, the roughness features were referred from existing literature, rather than handing over to ML models for automatic

determination. In addition, the scale of the dataset created from experimental and field studies is usually limited, so the model confidence level is low.

This study aims to establish data-driven PSS criteria of artificially-split rock fractures with high accuracy and strong universality. The dataset was composed of numerical specimens generated by direct shear test performed in particle-based discrete element method (PDEM), and fractures were randomly produced by diamond-square (DS) algorithm. Deep learning model convolutional neural network (CNN) was trained to automatically extract the fracture features, data augmentation and fine-tuning technique were also used to enhance the learning effect. It turned out to be effective in deep learning-aided prediction of fractured rock PSS.

2 METHODOLOGY

2.1 Dataset Preparation

2.1.1 Numerical modeling and fracture generation

Particle flow code PFC2D is used to construct a large-scale dataset of direct shear tests on numerical fractured specimens. Choosing 2D version is a trade-off between precision and time cost. The capability of PFC2D in simulating fracture shear behavior has been validated, and basic modeling procedure can be found in Zhao et al. (2019).

A few simulation tricks are utilized to improve computational accuracy and efficiency. First, a layered modeling method is applied (Zhao et al. 2012). Second, the dominated profile of fractures is determined by analysis of unweighted normalized associated roughness indicator. Third, newly-generated contacts between upper and lower blocks are mimicked by smooth joint model (SJM), which prevents the presence of lock up points and stress concentration (Figure 1), known as joint sides checking approach (Mehranpour and Kulatilake 2017).

DS algorithm is a widely used random midpoint displacement method based on fractal theory, to eventually shape a digital elevation model with roughness features similar to rock fractures in interest (Song et al. 2021). In this algorithm, standard deviation of normal distribution that elevation of coordinate points obeys (d), and reduced multiple of d after a diamond-square step (s), mainly dominate the macro and micro roughness respectively. Via adjusting these two parameters, the roughness features of generated random fractures can resemble those of real ones.

2.1.2 Dataset construction

In a round of simulations, micro-parameters remain unchanged to ensure the same rock type, and PSS of intact rock when σ =5MPa (τ_0), normal stress (σ), basic friction angle (ϕ_b), relative fracture elevation matrix (E) and corresponding PSS (τ) should be obtained. It indicates that direct shear test of intact rock, fractured rock with flat and rough surface, should be numerically conducted after rationality validation of PDEM. Noted that E is elevation of lower block surface, assuming the same shape of both blocks. The required dataset { $\tau_0, \phi_b, \sigma, E, \tau$ } can be obtained in plenty rounds of random simulations, then randomly split into the training set, validation set and test set (Wu et al. 2019).

Generally, numerical modeling of direct shear test excludes gravitational field, so theoretically the results ought to be the same when the entire model is rotated at any angle in plane. Considering the fractured specimen cannot be reused to verify the rotation equivalence, ten groups of dual tests (rotation angle is 180°) using PFC2D were conducted (Figure 1), and the relative error of each group was less than 5%, proving reasonability.

The above data augmentation technique has taken advantage of field prior knowledge as mentioned. Besides that, gaussian noise can also be added to fracture elevation as a universal augmentation technique to enhance generalization ability.

Furthermore, when φ_b and σ are already known but the model is incapable of telling the correct answer, obviously it is not robust. Feeding some samples of flat-surface fractures is necessary.

PDEM simulation results still have some difference with real tests due to particle flow hypothesis, belonging to low-fidelity data. Moreover, augmented data has lower fidelity apparently, and flat-

surface data is just to increase model robustness instead of improving PSS prediction accuracy of rough fractures, so the amount of new addition should be limited (Figure 1).



Figure 1. Dataset preparation. "LCM" means linear contact model, "BPM" means bonded-particle model.

2.2 Deep learning method

2.2.1 Convolutional neural network

Deep learning is algorithms that model high-level abstractions in data using architectures consisting of multiple nonlinear transformations. Training matrix data with fully-connected (FC) network will cause spatial information loss and parameter explosion. The 2D receptive field, local connectivity and parameter sharing strategies of CNN can solve this problem to some extent, and greatly increase convergence speed.

In convolution layers, trainable convolution kernels can automatically extract roughness features of fracture elevation at different levels. In pooling layers, down sampling is performed and feature dimension is reduced. Batch normalization (BN) is to make optimization landscape easier to explore, and activation function is to increase nonlinearity of network. When matrix is flattened, it will be combined with the other numeric features in this study, and reaching the output layer in the end after some FC layers. Some special techniques can be adopted according to specific requirement, such as dropout layer which randomly discard part of the nodes to improve stability and robustness, and attention which filters unimportant information and speed up convergence, or other specially-designed structures. Back-propagation algorithm is used to update weight and bias in epochs, until evaluation indicator on the validation set reaches our expectation. Performance on the test set determines the eventual score of the deep learning model.

2.2.2 Data preprocessing and model evaluation

To eliminate the influence of data dimension and ensure the scale consistency, numeric features and label need to be linearly scaled to the range of [0,1] by min-max scaling, while E need not since it'll go over batch normalization. All sets share the same minimum and maximum from the training set, because it's acquiescently regarded to be containing all relevant data in the world.

In order to comprehensively evaluate the prediction ability of the deep learning model, four evaluation indicators including root mean squared error (RMSE), mean absolute error (MAE), R-square (R^2) and mean absolute percentage error before normalization (MAPE) are selected to assess the error between true and predicted values (Wu et al. 2019). Trial-and-error method is used to search the optimal hyperparameter combination on the validation set. Evaluation indicators are not only used on the test set, but also on experimental data from this study and other researchers, to assess both the in-distribution and out-of-distribution generalization ability.

3 DATA-DRIVEN PSS CRITERIA OF ROCK FRACTURES

3.1 FracSNet

Granite from Qinghai Province and sandstone from Jiangxi Province in China were made into cubic rock specimens with a side length of 50 mm. Fractured specimens with flat surfaces were axially cut and polished, while those with rough surfaces were split by Brazilian tension. Surface morphology was measured by 3D laser scanner (OKIO-5M, TENYOUN), point clouds were linearly interpolated into a 256×256 square mesh, and the minimum elevation was subtracted. The direct shear test was performed with a servo-controlled shear apparatus YZW-100 (Li et al. 2020).

Numerical rock specimens were built up to mimic the three types of rock specimens, using tricks mentioned in 2.1.1. The relation curves of shear stress-shear displacement obtained experimentally and numerically match well (Figure 2), thus the rationality of PDEM in shear behavior simulation is successfully validated.



Figure 2. Experimental and numerical results of direct shear tests. "G" means granite, "S" means sandstone. Number 1-2 are intact rock, 3-4 are flat-surface fractured rock, and 5-6 are rough-surface fractured rock. In G-4 and S-4, σ=10MPa and 2.5MPa respectively, while 5MPa in the other cases.

Massive random fractures were digitized using DS algorithm with d and s valued in proper range, and the sampling interval was consistent with scanning results. In random simulations, the range of micro-parameters are referred from calibrated value range of two rock types and further extrapolated. In the end, 852 valid dataset samples were obtained, after running for two weeks on eight CPUs. The percentage of the training set, validation set and test set is 0.75, 0.10 and 0.15, respectively. When using data augmentation technique, each type of augmented data is 1/3 size of the training set.

The deep learning model named FracSNet was established on Tensorflow. Before feature concatenation is essentially embedding manipulation of matrix data. Except the top FC layer, activation uses rectified linear activation function (ReLU), to avoid gradient vanishing. Optimizer uses Adam. Learning rate is 0.0005 with a 10% decay every 100 epochs, and the batch size is 30. In 500 epochs with GPU acelerated, the best model was saved.



Figure 3. The structure of FracSNet.

3.2 Results

In this study, four types of deep learning models were developed and compared on the test set and experimental data:

- Multilayer Perceptron (MLP). Input features exclude *E*, as a blank group.
- FracSNet-v1. The training set is the original one without data augmentation.
- FracSNet-v2. The training set is enlarged with data augmentation in 2.1.2.
- FracSNet-v3. The training set is the same as FracSNet-v2, and fine-tuning is used.

To improve integrity of FracSNet and make it more reliable on the target rock type from other regions, fine-tuning is used on FracSNet-v3. In detail, first we utilize trained FracSNet-v2 as a pre-trained model, then freeze network parameters into untrainable state, replace the output layer with two FC layers to be trained, and feed in some target experimental data until reaching requirement at last.

Table 1 shows performance of the first three models on the test set. MLP is the worst for ignoring fracture roughness and meanwhile it proves contribution of convolution kernels. The prediction ability of FracSNet-v1 and FracSNet-v2 resemble each other, and outranks MLP.

Table 1. Model performance on the test set.

Model	RMSE	MAE	\mathbb{R}^2	MAPE
MLP	0.089	0.069	0.799	0.167
FracSNet-v1	0.029	0.021	0.979	0.047
FracSNet-v2	0.027	0.020	0.979	0.050

Note: It's meaningless to evaluate on the old test set for FracSNet-v3.

Figure 4 shows performance of the above models and classical Barton-Bandis (BB) model (Barton and Choubey 1977) on our (in 3.1) and additional experimental data (granite from Gansu Province, China). Joint roughness coefficient (JRC) is calculated according to Sun et al. (2013), which is independent of sampling interval. Prediction accuracy on additional data is lower due to different data source and distribution. MLP is completely unable to predict accurately because of bad performance on the test set, thus not shown in Figure 4. FracSNet-v1 has higher prediction accuracy than BB model on rough-surface data, indicating that it has mastered some more implicit roughness features. FracSNet-v2 assisted with data augmentation apparently has a global better prediction ability on both fracture types of rocks, and MAPEs (relative errors) of our flat-surface, rough-surface and additional rough-surface data are 7.6%, 1.9% and 19.3% respectively. FracSNet-v3 uses the last five target data (D12-S2) in addition with their augmented data to fine-tune weights of the untrained FC layers, an obvious decrease in MAPEs of additional data takes place, and the network still holds acceptable prediction ability on our experimental data. The corresponding MAPEs are 11.8%, 15.2% and 10.5% respectively.



Figure 4. Model performance on flat-surface samples, rough-surface samples and additional rough-surface samples in Zhao et al. (2019) and unpublished reports.

4 DISCUSSION AND CONCLUSION

A methodology of constructing data-driven PSS criteria of rock fractures is proposed in this study. Jointly using PDEM and DS algorithm to construct dataset breaks the limitation of dataset scale and improves the confidence. Use of CNN totally transfers the functionality of roughness feature extraction to models. Data augmentation detail is specified in this study, which can markedly improve accuracy. Use in combination with fine-tuning can help the model further approximate the true fracture PSS of target rock types. The data-driven PSS criteria of rock fractures would have a great potential in engineering application with limited access to experimental data.

In the future, deep learning is possibly applicable to fractures which are wet, with unfixed size and weathering and fillings. The selection of target experimental data for training needs balancing learning effect and users' convenience, and fine-tuning may be more mature in future studies. JRC of BB model is usually obtained by experimental inversion rather than forward calculation, so it is still reliable in estimating PSS of rock fractures.

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