PFC model parameter calibration using uniform experimental design and a deep learning network

Shijie Zhai¹, Jiewei Zhan¹, Yiding Bao¹, Jianping Chen¹,*, Yuchao Li¹, Zhihai Li¹

¹ College of Construction Engineering, Jilin University, Changchun, 130026, China
* Corresponding author. Tel.: +86 13843047952
* Email address: chenjp@jlu.edu.cn

Abstract. A macroscopic parameter calibration method for the particle flow code (PFC) using a uniform experimental design and deep learning network is proposed to explore the relationship between the micro parameters and macro response of rocks. First, a sensitivity analysis was used to identify which micro parameters influence the macro factors. A uniform experimental design was applied to achieve this goal in this study. Then, a neural network based on batch normalization was constructed. Through a large number of numerical simulation tests, the relationship between the input (micro parameters) and output (macro response) can be obtained by deep neural network (DNN). Finally, the DNN model was used to perform validation by using marble in Jining. The average error for the best results was only 4.211%. The main advantage of this method is that it can achieve fast parameter calibration compared with traditional calibration methods, and the calibration results can be obtained in only a few seconds through the designed program.

1. Introduction
The discrete element method (DEM), which is originated from molecular dynamics, is a powerful tool for analyzing the dynamics of material systems. In the DEM, the system is idealized as a whole and formed by the geometry of the structural elements. As one of the representatives of the DEM, the particle flow code (PFC) has been widely used in geotechnical engineering and geomechanical engineering. The basic principle of the PFC is derived from molecular dynamics. It was first proposed by Cundall [1] for a cohesionless granular material, and it can simulate rock by incorporating the bond particle model (BPM) [2]. The PFC attempts to reproduce the mechanical properties and behaviors of matter from a microscopic perspective. Before using the PFC for analysis, it is very important to establish the same model used for the actual material. However, due to the uncertainties in microscopic parameters and macroscopic responses, the calibration of macroscopic and microscopic parameters must be performed first. A widely used calibration method is the trial and error method. The biggest disadvantage of this method is that it is time consuming. Because the model parameter calibration directly determines the accuracy of the calculation, many scholars have studied this field. Yoon [3] studied the sensitivity and nonlinear relationship between micro parameters and macro parameters using the Plackett-Burman design method and statistical center composite design method. Hanley et al. [4] optimized the DEM calibration process by using the Taguchi method. Chehreghani et al. [5] used the response surface method and the central composite design method to calibrate the
BPM model. Castro-Filgueira et al. [6] specifically analyzed the sensitivity of microscopic parameters and macroscopic parameters for rock mass. Xia et al. [7] studied the relationships between the microscopic parameters of bedding planes and the macroscopic characteristics of transversely isotropic rocks using bonded-particle a discrete element model. Although these methods are much better than the traditional method, the calibration process is still complicated. In conclusion, the biggest problem of traditional calibration methods and these methods is that they will consume a lot of time to complete, and the accuracy cannot be guaranteed.

To address the limitations of traditional calibration methods, a new calibration method is proposed. The principle of this method is based on deep learning. Due to the development of computer technology, deep learning gradually gives full play to its advantages over traditional neural networks in finding rules from large amounts of data and establishing accurate models. In this paper, the purpose of this method is to quickly and accurately calculate the micro parameters required by the model according to the actual macro parameters of the input material.

The remainder of this paper is organized as follows: First, section 2 introduces the fundamentals of the BPM model, the uniform experimental design, and the deep learning model. In section 3, the methods mentioned in the second section are applied. Section 4 verifies the trained neural network. Finally, some conclusions are drawn in section 5.

2. Background

2.1. Parallel Bond Model

PFC3D is applied to carry out numerical simulation experiments. The selected BPM is a parallel bond model that can be regarded as a set of springs, with normal stiffness and shear stiffness existing in the contact bond of the particles. When the particles move relative to each other, tension and torque are generated. If these forces exceed the preset strength conditions, the bonds will break. A schematic diagram of the parallel bond contact model is shown in Fig. 1.

2.2. Uniform design experimentation

Experimental design is a branch of mathematical statistics. It is about making appropriate experimental plans and realizing the effective analysis of experimental results.

The uniform design method was proposed by Fang and Wang in 1978. The uniform design method is a multifactor and multilevel method in experimental design. Its mathematical principle is to replace the complete combination of all possible experimental parameters by a small number of experimental trials uniformly distributed within the parameter space [8, 9]. Through this design method, the test points can be completely and evenly dispersed within the experimental range, resulting in each point having better representativeness [10, 11, 12]. Uniform test design has obvious advantages over orthogonal test design. It can accomplish the same thing but with fewer trials as orthogonal trials. For example, in an experiment with n levels, the orthogonal experiment needs to carry out n^2 experiments, while the uniform design needs to carry out at least n experiments [13].

The table used for uniform design is called a uniform design table [14], which can be divided into an equal horizontal design table and a mixed level design table.

2.3. Deep learning

Deep learning originates from machine learning. The typical structure of networks is composed of multiple layers and units. These layers include an input layer, an output layer and one or more hidden layers. Each layer is composed of some number of units. Data are passed from the input layer to the output layer. The input from each unit in the previous layer is multiplied by a weight. In each unit, the weighted input values are summed and added with bias. This combination of inputs then generates the output of the unit through a nonlinear activation function. The process can be expressed by the following equation.

\[ y = f(\omega^T x + b) \quad \omega = (\omega_1, \omega_2, \ldots, \omega_n) \]
In the process of training, in order to make the model more accurate, the error rate is calculated and the error is transmitted back after a training. This process is called back propagation algorithm (BP). Fig. 4 (b) shows the schematic of a neuron. The flow chart of this design is shown in Fig. 2.

3. Methodology

3.1. Acquisition of macroscopic responses

The macroscopic response of the model is obtained by a simulation test. To more accurately reproduce the properties of the actual material, five macroscopic responses are used for calibration. Their values are obtained from stress-strain curves derived from the simulated experiments. The values of each macroscopic response are shown in Fig. 3.

3.2. Application of uniform design

The homogenous mixture design table is used for the experimental design of the sensitivity analysis. The uniform design depends on the regression analysis method to parse the results. Eight microscopic parameters are selected to analyze the sensitivity of five macroscopic responses, and the remaining microscopic parameters are specified. The horizontal division of each microscopic parameter is shown in Table 1.
Table 1 Microscopic parameter level.

| parameters          | level          |
|---------------------|---------------|
| \( r_{\text{min}} \) | 0.9 1 1.3 1.5 |
| \( ba_{\text{rho}} \) | 2100 2200 2300 2400 2500 2600 2700 |
| \( pb_{\text{Ec}} \) | 20 40 60 80 100 120 140 |
| \( pb_{\text{krat}} \) | 1 2 3 4 |
| \( pb_{\text{sn_mean}} \) | 30 35 40 45 50 55 60 65 70 75 80 85 90 95 |
| \( pb_{\text{coh_mean}} \) | 100 105 110 115 120 125 130 135 140 145 150 155 160 165 |
| \( pb_{\phi} \) | 5 7 21 27 33 39 45 |
| \( ba_{\text{fric}} \) | 0.1 0.13 0.16 0.19 0.22 0.25 0.28 0.31 0.34 0.37 0.4 0.43 0.46 0.49 |
| \( pb_{\phi} \) | 0.52 0.55 0.58 0.61 0.64 0.67 0.7 0.73 0.76 0.79 0.82 0.85 0.88 0.91 |

Regression analysis was performed according to the results, as shown in Table 2. According to the results, the micro parameters that have a great impact on the macro response are \( pb_{\text{Ec}} \), \( pb_{\text{krat}} \), \( pb_{\text{sn_mean}} \), \( pb_{\text{coh_mean}} \), and \( pb_{\phi} \).

Table 2 Regression analysis results.

| Factors            | Y1 | Y2 | Y3 | Y4 | Y5 |
|--------------------|----|----|----|----|----|
|                    | coeff | p    | coeff | p    | coeff | p    | coeff | p    | coeff | p    |
| Constant           | -141.924 | .270 | 186.677 | .098 | -.058 | .634 | -45.144 | .214 | 27.178 | .017 |
| \( r_{\text{min}} \) | 2.215 | .943 | -.9073 | .732 | .014 | .636 | 3.873 | .655 | -1.644 | .522 |
| \( \rho \)        | .050 | .211 | -.962 | .078 | 7.778E-5 | .052 | .015 | .180 | -.001 | .873 |
| \( pb_{\text{Ec}} \) | .128 | .499 | .743 | .000 | .000 | .109 | .059 | .276 | -.028 | .082 |
| \( pb_{\text{krat}} \) | -5.777 | .449 | 1.334 | .837 | .034 | .000 | -2.523 | .244 | 1.081 | .097 |
| \( pb_{\text{sn_mean}} \) | .520 | .015 | .168 | .327 | -6.803E-5 | .722 | .179 | .004 | -.036 | .040 |
| \( pb_{\text{coh_mean}} \) | .635 | .003 | .049 | .766 | -2.684E-5 | .885 | .156 | .008 | .056 | .002 |
| \( pb_{\phi} \)   | .282 | .598 | -1.049 | .031 | .001 | .065 | .020 | .891 | .119 | .013 |
| \( ba_{\text{fric}} \) | 19.944 | .533 | -5.400 | .843 | -.041 | .190 | 5.407 | .547 | 4.658 | .090 |

3.3. Application of the DNN

3.3.1. Network construction. Pytorch, an open source framework for deep learning, is adopted to establish a DNN through programming for this research. The network structure is shown in Fig. 4 (c). In addition, we need to set up the activation function when constructing the DNN model. The ReLU function is generally selected by the DNN model, as shown in Fig. 4 (a). To update the network parameters, an optimizer is used. The loss function used in this network is the mean square error (MSELoss). The equation is shown below.

\[
\text{MSELoss} = \frac{1}{n} \sum_{i=1}^{n} (l_i - l_{\text{actual}})_i^2, \quad l_i = (x_i + y_i)^2
\]  

(2)
3.3.2. Data preprocessing. A total of 288 sets of numerical simulation tests were conducted on different microscopic parameters (as outputs) through PFC3D. The macroscopic responses (as inputs) are obtained through data processing. Thirty percent of the data are used as test sets to evaluate the performance of the network so that the DNN model has better generalization ability. Data preprocessing is very important before training the neural network; therefore, min-max normalization is used to preprocess the data.

3.3.3. Parameter tuning and training. Some hyper parameters need to be set before carrying out the training network. Learned models are often significantly different with different parameter configurations. Therefore, the hyper parameters also need to be set, as does the algorithm. The mean square error is used as a performance measurement method in this paper. The evaluation method adopts the hold-out method, that is, 30% of data are selected as the test set to evaluate the test error of the network and estimate the generalization error.

The results of hyper parameter tuning are shown in Fig. 5, and the hyper parameter with the lowest loss is selected. The learning rate, number of units, data volume of each mini batch and number of layers are 0.002, 16, 64 and 16, respectively. After tuning the parameters, the network can be trained. The mean square error is selected as a performance measure. The mean square error graph of the network is shown in Fig. 6.

4. Verification of the network
To verify the performance of the neural network, marble from the Jinping hydropower station is selected as the calibration object. The specific values are shown in Table 3.
Table 3 Laboratory test result and simulation result.

| Property                  | Laboratory test | Simulation results | Relative error |
|---------------------------|-----------------|--------------------|----------------|
| Unconfined compressive    | 77.3            | 68                 | 12.031%        |
| Young’s modulus (GPa)     | 85              | 67                 | 21.176%        |
| Poisson’s ratio           | 0.26            | 0.28               | 9.615%         |
| Cohesion strength (MPa)   | 26.8            | 19.3               | 27.985%        |
| Internal friction angle (°)| 27.1            | 30.549             | 12.726%        |
| **Average error**         |                 | 16.714%            | 4.211%         |

As seen from the tables, the macroscopic response of the model with the parameters calculated by the neural network is mostly consistent with the expected macroscopic response. The average error of the second group is only 4.211%, which accurately reflects the nature of the material.

5. Conclusions
The results show that this neural network can calibrate the PFC3D model well and has the advantages of high speed and accuracy. However, some individual macro responses are not very accurate. To solve this problem with the improved model, a large amount of training data needs to be added in the future.

Acknowledgments
This work was supported by the National Natural Science Fund of China (Grant No. 41330636), by the National Natural Science Foundation - Yunnan joint fund key support project (Grant No. U1702241).

References
[1] Cundall, P.A. A Computer Model for Simulating Progressive Large Scale Movements in Blocky Rock Systems. Proceedings of the Symposium of the International Society for Rock Mechanics, Society for Rock Mechanics (ISRM), France, II-8.
[2] D.O. Potyondy, P.A. Cundall. A bonded-particle model for rock International Journal of Rock Mechanics & Mining Sciences 2004; 41:1329–1364.
[3] Jeoungseok Yoon. Application of experimental design and optimization to PFC model calibration in uniaxial compression simulation. International Journal of Rock Mechanics & Mining Sciences 2007; 44: 871–889.
[4] Kevin J. Hanley, Catherine O’Sullivan, Jorge C. Oliveira, Kevin Cronin, Edmond P. Byrne. Application of Taguchi methods to DEM calibration of bonded agglomerates. Powder Technology 2011; 210:230-240.
[5] Sajjad Chehreghani, Mohammad Noaparast, Bahram Rezai, Sied Ziaedin Shafaei. Bonded-particle model calibration using response surfacemethodology. Particuology 2017; 32: 141–152.
[6] U. Castro-Filgueira, L.R. Alejano, J. Arzúa, D. Mas Ivars. Sensitivity Analysis of the Micro-Parameters Used in a PFC Analysis Towards the Mechanical Properties of Rocks. Procedia Engineering 2017; 191: 488 – 495.
[7] Lei Xia, Yawu Zeng. Parametric study of smooth joint parameters on the mechanical behavior of transversely isotropic rocks and research on calibration method. Computers and Geotechnic 2018; 98: 1–7.
[8] Gu Song, Guoqiang Xu, Yongkai Quan, Qingchun Yuan, Philip A. Davies. Uniform design for the optimization of Al2O3 nanofilms produced by electrophoretic deposition. Surface & Coatings Technology 2016;286: 268–278.
[9] J.F. Li, et al. Uniform design method for optimization of process parameters of plasma sprayed TiN coatings. Surface and Coatings Technology 2003; 176:1–13.
[10] K.T. Fang, Y. Wang, Number-Theoretic Methods in Statistics, Chapman and Hall, London, 1994, ISBN 0412465205.
[11] K.T. Fang, The uniform design: application of number-theoretic methods in experimental design, Acta Math. Appl. Sin. 1980; 3: 363–372.
[12] K.T. Fang, D.K.J. Lin, P. Winker, Y. Zhang, Uniform design: theory and application, Technometrics 2000; 42: 237–248.
[13] WU Jie, ZHU fei, XU Jing. Optimization on the Extraction of Polysaccharides from Fructus Corni Using Uniform Design. Procedia Engineering 2011; 24:484-489.
[14] Jintao Guan, et al. Optimizational production of phenyllactic acid by a Lactobacillus buchneri strain via uniform design with overlay sampling. Chinese Journal of Chemical Engineering 2018.