An example of calibrating physical parameters in a constitutive model based on machine learning framework

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ABSTRACT: In order to more accurately describe the behavior of geological materials, constitutive models with increasing complexity are being developed. The increase in the number of parameters and equations makes engineering applications difficult. On the other hand, data-driven machine learning approaches have shown great potential in addressing this issue. Therefore, from a data perspective, this paper recapitulates and discuss the task and framework of machine learning. For the parameter calibration task, 1-Dimensional Convolutional Neural Networks (1D-CNN), Recurrent Neural Network (RNN), Genetic Algorithm (GA), and Particle Swarm Optimization (PSO) were tested under the framework of representation learning and optimization. In the preset computing environment, the normalized RMSEs of representation learning are 0.21 and 0.17, and the calculation takes less than 0.1 second. Optimization frameworks perform better with RMSEs of 0.04 and 0.07, but cost over 10 hours. Finally, the advantages and disadvantages of each framework are discussed.

Keywords: Machine Learning. Constitutive Model. Parameter Calibration. Representation.

1 INTRODUCTION

The mechanical behavior of geomaterials is often observed with nonlinear laws which have been shown to involve structural properties, anisotropy, saturation, temperature, chemistry, and time dependence. These complex stress-strain relationships, which are usually systematically and controllably generalized by laboratory element experiments, are mathematically described as constitutive model. Using constitutive model under geometric and mechanical boundary conditions, it is feasible that establish numerical simulations for solving engineering problem. In order to provide high quality computational simulations and recommendations in specific geological conditions, researchers have been exploring and creating new constitutive models to more accurately describe geological materials. In the past few decades, from the original perfect linear-elastic model, it was developed to include more accurate critical state models for complex geological states. However, there are still several issues that limit the development and application of constitutive models: 1) As the mathematical formulation becomes complex, the parameter calibration of the constitutive model is very cumbersome causing difficulties in application. 2) Many models are proprietary only for specific geological conditions and show low applicability to other geological conditions.

Recently, artificial intelligence approaches have received a lot of attention. A number of scholars are also exploring the potential of machine learning (ML) methods in describing geomaterials constitutive relationships. Zhang (2020) used Long Short-Term Memory (LSTM) to take each state of the soil as input variables and gave the mechanical properties behavior of Toyoura sand under both drained and undrained conditions. Qu (2021) used gated recurrent unit (GRU) networks to predict the stress responses of granular materials subjected to a given unseen strain path. However, this approach of creating constitutive relationships based on machine learning has two limitations. 1) The element experiments in the laboratory are time-consuming and costly, resulting in only a small amount of data for ML training, which makes the ml-based constitutive relationship often manifest as weak generalization ability and overfitting. Whereas most researchers use the data set of element numerical simulation, but the ML model trained with the simulated data will never show better performance and dig deeper mechanisms than the constitutive model of the data source. 2) Second, the " time-series prediction constitutive relationship" constructed by neural networks has higher computational complexity, and it is difficult to be discretized in space and calculate practical engineering problems. In summary, the essence of machine learning is to mine the inherent laws of data. Therefore, this kind of machine learning method that ignore the original physical model will not bring new knowledge. It is necessary to combine machine learning and constitutive models.

This paper summarizes three machine learning frameworks based on the constitutive model, representation learning and optimization methods, and time-series prediction. In the subsequent discussion, two kinds of representation learning, 1-Dimensional Convolutional Neural Networks (1D-CNN), Recurrent Neural Network (RNN), and two optimization methods such as Genetic Algorithm (GA), and Particle Swarm Optimization (PSO) were used to solve the task of the same parameter calibration. Finally, the application potential of ML methods is discussed.

2 MACHINE LEARNING FRAMEWORK

It is well known that the key to the ability of machine learning to solve real-world problems lies in the quality of the data-set and the applicability of the methods. Therefore, it is worthwhile summarizing the data source and machine learning tasks in a new data-perspective, which helps to address more clearly the issues encountered with the constitutive mode. As shown in Figure 1, the constitutive model is reclassified into three types of information input, output, and function computation. Based on these three types of information interactions, here are three different frameworks for machine learning: 1) Time-series prediction; 2) Representation learning; 3) Optimal search.

2.1 Information from constitutive model

A constitutive model is a mathematical representation that describes the behavior of a material under different conditions of stress, strain, temperature, and other factors.

The input data can be divided into the following categories. a) Initial state. For geological materials, it contains initial pore space, initial atmospheric pressure, initial temperature, initial saturation, over consolidation ratio, etc. b) A stress path, refers to the path followed by a material in the stress space as it undergoes deformation or loading. Rates are also included in the calculation of the constitutive relations, which eventually discretize the loaded deformation or stress for each step. c) Physics parameters. For geological materials, it generally comes from the inherent properties of the material. Such as Poisson's ratio, Compression index, Swelling index, Critical state parameter, etc. d) Mathematical assumption parameter. Which are obtained statistically and may have no real physical meaning in order to satisfy mathematical calculations. An example is the coefficient describing the shape of the yield surface.

The second part is the calculation of the constitutive model. Their calculation methods are generally obtained from laboratory experiments, and are mathematically summarized as the response of the initial state under the input stress and strain conditions. For example, under the elastic-plastic theory, in each step of calculation, according to the current state of the material, the yield surface function and flow law in the stress space are used to identify and calculate the magnitude and direction of the plastic deformation of the material. After obtaining the plastic behavior response, the calculation and output is the state at the next step. Then the next-step state will be calculated cyclically as the new initial state.

The output part is the state of each step calculated by the constitutive model for a material, which depends on the input data, the initial state of the material and the loading path. These results will be used to solve practical problems. For example, in laboratory element experiments, the same stress paths are loaded on the unit material by the triaxial tester. The actual response state of the specimens will be used to determine whether the constitutive relationship is accurate. On the other hand, in the numerical simulation of finite element method for geological engineering, each discrete element will also get the mechanical response of each state at each step, which is used to analyze engineering boundary problems.

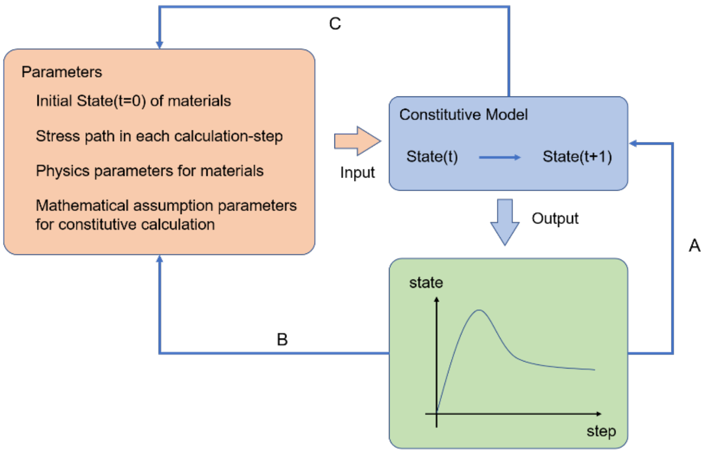

Figure 1. The machine learning frameworks for constitutive model. Three boxes indicate the data and functions required for the computation in constitutional model. Arrows (numbered A-C) indicate possible tasks and goals for machine learning A: Time-series prediction; B: Representation learning; C: Optimal search.

2.2 Time-series prediction

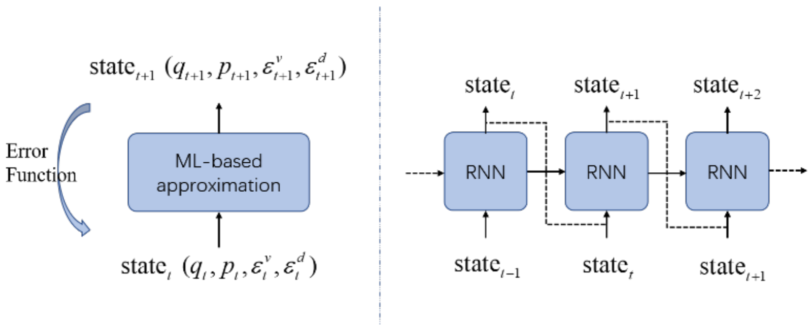

Figure 2. Time-series prediction task (left) and Recurrent Neural Network structure (right) for cam-clay.

Information flow A in Figure 1 is considered as a time series forecasting task. It is obvious that the output of constitutive relations is a time-dependent sequence of states. Time series forecasting refers to the establishment of approximate models for constitutive functions by machine learning through the historical sequence of these state transitions. After the training is completed, the algorithm realizes the input of the current state and stress conditions, and the output is the prediction result of the next moment. The state of the art are mainly based on recurrent neural network modeling, including LSTM, GRU, etc. Figure 2 gives the task definition and general neural network structure for the cam-clay model. This framework is used in many ML-based constitutive models(Chen et al. 2022; Meng and Pei 2023). Since most of the gradient information is derived from the time-varying state of the material, the generalization capability will also be limited to nearby stress paths and similar materials.

2.3 Representation learning

The goal of representation learning is to find a more compact and meaningful representation of the input data that captures the important information and structure in the data. Information flow B in Figure 1 is considered as a representation task. That is, the input parameters of the constitutive model are represented by the observed material state sequence. This structure sidesteps the calculation of constitutive relations and becomes an encoding and decoding problem. Figure 3 shows the tasks used for representation learning. Some machine learning algorithms could be employed such as 1D-CNN RNN and Transform. This framework is more common in some geotechnical fields for boundary problems - predicting boundary conditions from the state curve of one point (S. Zhang et al. 2022; Ishitsuka et al. 2021).

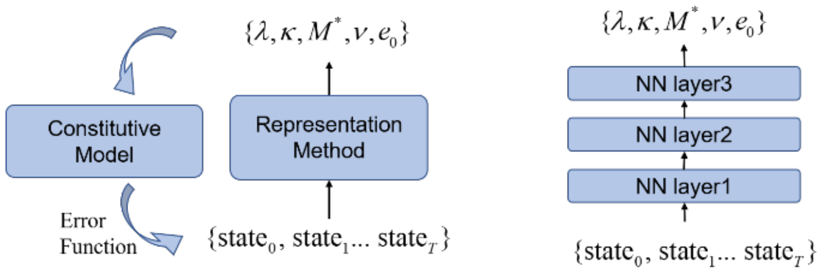

Figure 3. Representation learning task (left), Structure diagram (right). NN layer represents the basic modules of the neural network, including convolution, fully connected modules, attention modules, etc.

2.4 Optimization

Optimization refers to the process of finding the best possible solution to a problem, given certain constraints and objective criteria. For the task described in Figure 1, it is to find the optimal input parameters of the constitutive model to match the expected material behavior. This means that the parameters are defined in a search space, and the maximum optimization objective. In order to avoid falling into the local optimal solution, some bionic optimization algorithms, such as Genetic algorithm and particle swarm optimization algorithm are often used. Figure 4 shows the application of cam-clay model parameter search. Because of the need for a well-defined search space, this framework is often used for parameter calibration. (Levasseur et al. 2008; Yin et al. 2017)

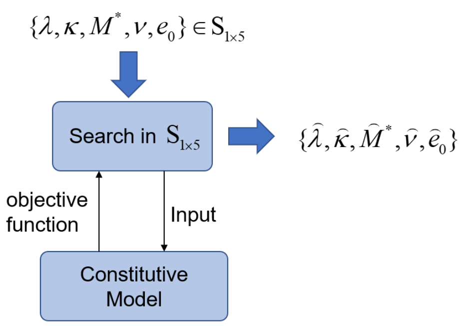

Figure 4. Optimization frameworks using constitutive model.

3 PERFORMANCE ON CALIBRATION PARAMETER TASKS

3.1 Calibration Parameter Task

The same parameter calibration task is given to discuss machine learning frameworks (representation learning and optimization methods) involving constitutive models. The composition of the data set is Toyoura sand standard parameters, which are obtained from Zhang's research (2010), as well as the results of element simulations given at arbitrary points in the parameter space. The task is described as inversion of the parameters used in the model from the simulated deviatoric stress - axial deformation curves of Toyoura sand. It is worth noting that the five parameters are all normalized to a smaller range, taking into account the order of magnitude difference of each parameter. Table 1 shows the values of the parameters.

Table 1. Calibration parameters task for Toyoura sand.

Parameter Name	Value	Search Space	max-min normalization
Compression index	0.05	(0.02, 0.07)	0.6
Swelling index	0.0064	(0.001,0.01)	0.6
Critical state parameter	1.30	(1.00,1.60)	0.5
Void ratio	0.87	(0.5,1)	0.74
Poisson's ratio	0.3	(0.1, 0.5)	0.5

For the machine learning model, two models of representation learning are employed. 1DCNN contains two fully connected layers with two convolutional layers and one pooling layer. The recurrent unit of RNN does not contain logic gate components. All neural networks are trained with the Adam optimizer on 10,000 sequences randomly generated in the parameter search space. The optimization algorithm includes GA and PSO. GA contains 140 initial populations, and the preset Swarm size of PSO is 160. All programs are programmed in python and calculated in intel core i7-9750H.

3.2 Results and discussion

Table 2. Comparison of models.

Model Name	RMSE (5 para)	RMSE (1-para)	Time (5-para)	Time (1-para)
1DCNN	0.21	0.04	<0.01s	<0.01s
RNN	0.17	0.05	<0.01s	<0.01s
GA	0.04	0.005	15h	13h
PSO	0.07	0.003	21h	11h

The RMSE of all prediction parameters and Toyoura sand parameters is used as the evaluation standard. In addition, the time for each model calculation is also recorded. It is worth noting that each model was tested twice, predicting all five parameters and only one of them. The optimal prediction results of all models are shown in Table 2. The performance of representation learning is worse than optimal search, but the optimization algorithm consumes more time. This may be caused by two reasons. First, all network parameters of the artificial neural network are updated according to the gradient. When the relationship between input and output is not mathematically smooth enough, the gradient update efficiency of the neural network will be reduced. On the other hand, the updates of GA and PSO though also depend on the gradient of the error. But because they have seeds for the initial search in the entire parameter space, the probability of falling into local optimum is low. Therefore, the results of all algorithms show better performance when the computational complexity is reduced, i.e. predicting only one parameter. Second, the artificial neural network establishes parameter characteristics through state curves, and what is established is still a one-to-one mapping relationship. But the optimal search algorithm is to select the optimal individual among multiple groups of search results in the exploration space. Since the calculation of each seed re-uses the constitutive relationship, the calculation time will be greatly increased.

4 CONCLUSION

From the perspective of data, this paper systematically summarizes several machine learning computing frameworks related to constitutive models. Then a simple comparison was made with the parameter calibration problem of Toyoura sand under the cam-clay model. Numeral experiments show that as the target parameters increase, the generalization ability of the general representation learning neural network adopted for the constitutive model is not good, but the exploration speed is fast. The optimized search algorithm works better but takes longer times. Considering that complex constitutive model are far more than the five parameters employed by experiments, new neural network structures need to be explored and developed under the proposed machine learning framework.

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