



RESEARCH ARTICLE

**AN EFFICIENT CALIBRATION PROCESS FOR THE PREDICTION OF ROCK
STRENGTH THROUGH MACHINE LEARNING ALGORITHMS**

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ABSTRACT

Numerical models based on the discrete element method (DEM) have been widely used to predict the mechanical behaviors of rocks in rock engineering applications. Nevertheless, calibration of the model parameters is done by running numerous simulations and this time-consuming simulation process precludes the numerical platforms to be used as a practical tool in such applications. This study aims to accelerate the calibration process of the micro-parameters of three-dimensional (3D) numerical models built based on DEM and facilitate the generation of an efficient database by using machine learning algorithms in the prediction of rock strength. Namely, these algorithms are linear regression (LR), decision tree (DT) regression, and random forest (RF) regression. The appropriate methodology for predicting the uniaxial compressive strengths (UCS) of certain rock types was investigated using a dataset consisting of micro-parameters of 87 DEM-based rock models, generated through an open-source code, Yade. The performance of such methods was evaluated by using metrics including R-squared score (R^2), mean squared error (MSE), root mean squared error (RMSE), and mean absolute error (MAE), and then their statistical discrepancies were analyzed. The most accurate prediction of UCS was obtained in the LR method and the lowest percentage of performance was derived from the RF algorithms. LR method provides the results efficiently during calibration of the micro-parameters of a DEM-based rock model.

Keywords: *Rock strength, Discrete element method, Numerical model calibration, Machine learning.*

1. INTRODUCTION

Determining the failure and deformation processes of rocks under applied stresses has paramount importance in rock engineering. While laboratory and analytical methods are used conventionally to investigate this process, recently numerical modeling methods have also been commonly used as an alternative/supporting and effective technique to these methods. In particular, for discontinuous media such as in rocks, numerical models based on the discrete element method (DEM) are mainly preferred because of their advantage in reflecting each structural element (e.g. cracks, joints, faults, layers, etc.) formed by rock behaviors. Therefore, deformation and damage processes examined through numerical modeling, provide useful insights into understanding the extent and magnitude of rock failure

characteristics [1-13]. On the other hand, the generation of a numerical model as a representative of the real rock domain depends on the accurate and reliable calibration of the model parameters. The calibration is done according to the fundamental macro mechanical parameters (i.e uniaxial compressive strength, UCS; tensile strength UTS, Young modulus, E and Poisson's ratio, ν) of the rocks obtained by laboratory experiments. As a result, in order to rely on precise calibration, numerous simulations are sometimes required to be run, and each simulation cycle can turn into a very time-consuming workload depending on the resolution of the generated model.

Machine learning (ML), one of today's artificial intelligence technologies, has become an established technique to produce objective and sensitive results within the most efficient timeframe for the problems encountered in energy & mining industries, as well as agriculture, finance, education, and many other fields. This technology facilitates targeted decision-making or forecasting by focusing on building systems that learn and improve performances based on the data type. Therefore, various machine learning methods have been developed according to the specific application topic, the purpose of the study, and the type of database. The most well-known and widely used methods for numerical datasets (e.g. integer, float, etc.) are artificial neural networks (ANN), linear regression (LR), decision trees (DT), Naive Bayes (NB), K-nearest neighbors (KNN), and random forest (RF) algorithms. Specifically, ANN has been considered in many studies that aim to predict one of the most critical parameters in rock engineering, for instance, the UCS value for revealing the effects of various rock properties [14- 26]. Furthermore, these studies [14-26] emphasize the important role of laboratory and field measurements and observations regarding rock failure characteristics.

Nevertheless, machine learning attempts on constituting efficient datasets and receiving quick responses from numerical modeling in rock deformation which is a robust tool for considering the scale effect, have rarely been used [27, 28, 29]. More specifically, machine learning studies focusing on the improvement of the calibration process of the DEM-based model parameters to achieve more productive and cost-efficient predictions for the rock strength and failure/deformation behaviors are very limited [28, 29]. For instance, Waqas [28], used machine learning techniques to provide a faster computational time in the discrete analysis of rock properties. However, the results may not be easily evaluated because of using only two metrics to measure the performance of the applied machine learning method. More recently, considering several statistical metrics to test the accuracy of the performances of the predictive models, Fathipour-Azar [29] estimated the UCS values of DEM-based models through machine learning approaches. UCS values were predicted according to two micro-shear properties, cohesion and internal friction angle of discrete elements' contacts. These attempts made by Fathipour-Azar [29] proposed a rapid calibration process through the utilized methods whose robustness might further be increased by using more input parameters.

In this study, LR, DT, and RF methods of machine learning technology were applied to the micro-parameters of three-dimensional (3D) numerical rock models based on DEM by considering the time, storage space, and optimization of the data processing, and thereupon, rock strength (UCS) values were predicted. The dataset has 87 rows and 7 columns consisting of 6 micro-parameters and UCS values that were derived from the numerical models assigned in accordance with these parameters. As the most common split ratio, 80% of the dataset goes into the training set and 20% of the dataset goes into the testing set. The performances of the methods were evaluated through the coefficient of

determination (R^2), mean squared error (MSE), mean absolute error (MAE), and root mean squared error (RMSE) metrics. The results present findings that contribute to the users acquiring data much faster in rock engineering applications where the DEM modeling technique is used.

2. METHODOLOGY

2.1. 3D-DEM Rock Model

The numerical rock models used in this study were generated using a 3D open-source DEM code, Yade [30]. It is fundamentally based on the bounded particle model (BPM) which was first proposed by Potyondy and Cundall [3] and then modified by Scholtès and Donzé [9] to be used in the DEM platform. A rock material is a structure/assembly consisting of bonded, rigid, and spherical particles of different sizes (Figure 1a). Particles are also called discrete elements (DEs) and these elements are bonded together (Figure 1b) in an interaction ratio (γ_{int}) based on the elastic-brittle contact law (Eq.1). This ratio is determined before the numerical model is generated.

$$D_{eq} \leq \gamma_{int} * (R_x + R_y) \quad (1)$$

Here, γ_{int} is the parameter that controls the initial number of interacting bonds (N). D_{eq} is the initial distance between the particles x and y with radii of R_x and R_y , respectively. This parameter as irrespective of the number of particles in the rock model is assigned before the simulation starts. It represents the average number of bonds per particle (N). Therefore, the rigidity of rock is controlled by decreasing or increasing the γ_{int} (or N) value according to the ratio of UCS to UTS of relevant rock material. For instance, for modeling a relatively weak rock material, γ_{int} is selected to be close to 1 which shows poor interlocking among the particles. Moreover, the greater γ_{int} values ($\gamma_{int} > 1$) indicate a rock with a higher UCS/UTS ratio and a more rigid domain (see Scholtès and Donzé [9] for more details).

Interaction forces between particles are subdivided into two components such as normal (F_n) and shear (F_s) forces (Figure 1c). Along the normal axis, F_n is calculated;

$$F_n = k_n * u_n \quad (2)$$

with k_n , the normal stiffness computed as a function of an equivalent elastic modulus Y (in Pa) (Eq. 3), and u_n is the normal relative displacement.

$$k_n = 2Y * \frac{R_x * R_y}{R_x + R_y} \quad (3)$$

Under compression, F_n can increase indefinitely while under tension, F_n increases up to a threshold value, $F_{n,max} = t * A_{int}$. Here, t is the interparticle tensile strength (in Pa), and A_{int} is the surface area that depends on the particle sizes ($A_{int} = \pi * [\min(R_x; R_y)]^2$). When $F_n \geq F_{n,max}$, the bond breaks, and a mode I (tensile) crack forms at the bond location.

F_s as the driving force along the shear axis is computed incrementally from the equation of $F_s = F_{s, t-\Delta t} + k_s \cdot \Delta u_s$. k_s is the shear stiffness obtained from $k_s = P \cdot k_n$ (Figure 1b). P is a model constant and it varies between 0 and 1. Δu_s is the relative incremental displacement and $F_{s, t-\Delta t}$ is the shear force at the previous timestep. So, the maximum admissible shear force, $F_{s, \max}$ is determined by Mohr-Coulomb criteria such as;

$$F_{s, \max} = c \cdot A_{\text{int}} + F_n \cdot \tan(\varphi) \quad (4)$$

where c is the interparticle cohesion (in Pa) and φ is the interparticle friction angle (in °). When $F_s \geq F_{s, \max}$, the bond breaks and a mode II (shear) crack forms at the bond location.

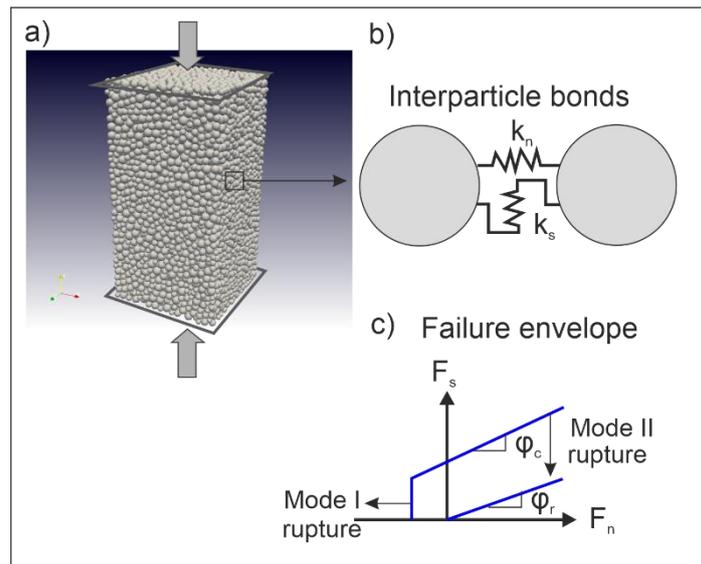


Figure 1. a) Configuration of 3D-DEM model sample (based on BPM technique) under UCS test simulation, b) Interparticle bonds, c) Interaction forces between the particles and rock failure mechanisms (modified from Scholtès and Donzé [9]).

It is worth noting that similar to the laboratory experiments, all simulations here were carried out under quasi-static conditions. Moreover, a global viscous damping ratio, chosen as 0.4 was used to reduce the kinetic energy during the simulations.

The parameters (Y , P , t , c , φ , and N) mentioned above are the micro-parameters of a 3D numerical DEM model and calibrated according to the macro mechanical strength parameters (UCS, UTS) and deformation parameters (E , Young modulus, and ν , Poisson's ratio) by performing a series of laboratory test simulations. The calibration process is repeated until the model represents accurately the stress-strain behaviors and mechanical properties of the real rock. Therefore, this process may take

longer and it requires many iterations and simulations. The type of simulation (tensile strength test, uniaxial compressive strength test, triaxial compressive strength test, etc.) is selected according to the parameter to be calibrated. For example, t as the tensile strength of the particles controls the UTS value and is derived from the UTS test simulation [12]. Furthermore, the calibration of some model parameters is done by running various test simulations. For example, c affects the UCS value while Y directly controls the E value of the rock material. P as the ratio of k_s to k_n has an influence on ν value of the rock. To calibrate these three macro-parameters, both uniaxial and triaxial compressive strength test simulations are required to run. ϕ controls the slope of the rock failure envelope and is determined directly in the triaxial compressive test simulations. As is different from others, the N parameter is assigned according to the UCS/UTS ratio of the real rock before the simulation starts. The details of the effects and roles of each micro-parameter on macro mechanical properties can also be followed in Dinç Göğüş [31].

Similar to other numerical rock modeling techniques, the duration of the calibration of a numerical DEM model is primarily dependent on the resolution of the generated model. For the sake of clarity and reducing complexity, all rock models here were built in $1 \times 2 \times 1$ model unit sizes and they consist of 10,000 particles to obtain the results to be irrespective of the model resolution.

The dataset used in the study has 87 rows and 7 columns consisting of 6 micro-parameters (Y , P , t , c , ϕ , and N) with different values as well as the UCS values (as the peak/maximum stress that the model can resist) of the 3D-DEM model samples formed by such parameters (Figure 2). The parameters belong to 6 different rock types, from the weak to the strong rock material: claystone, ignimbrite, marble, andesite, diabase, and granite.

The details of the machine learning methods on the dataset are given in the following section.

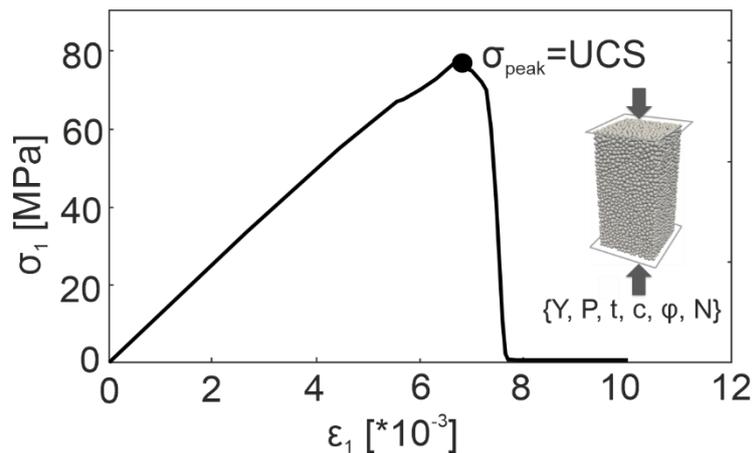


Figure 2. Under the uniaxial loading condition, the stress-strain response of a 3D-DEM model sample formed by 6 micro-parameters.

2.2. Machine Learning Methods

Machine learning, which teaches the existing data or information to the machine and extracts a function from this information is a subfield of artificial intelligence systems. The term machine learning was first introduced to the literature by Arthur Samuel an IBM employee, in 1959, and has been implemented in geotechnical and rock mechanical applications since the 1990s. The operation of the system, in which training data sets are used to obtain the targeted results and the user does not need to control the model, is based on the principle of using a known input dataset (training data). Further, the corresponding outputs are used to produce the most appropriate outputs for the new data (test data) that the algorithm has never seen before. (Figure 3). The flow chart of the machine learning process is presented in Figure 3. In this study, 20% of the total data is used for testing, and the remaining 80% is applied for training.

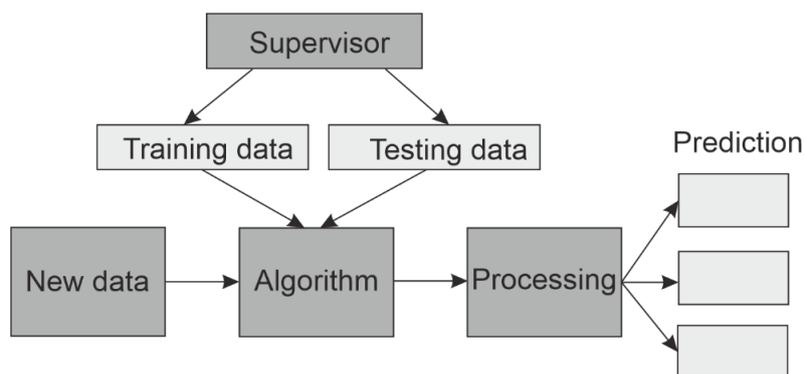


Figure 3. The general flow chart of the machine learning process.

The process of applying machine learning methods to the dataset consists of 3 stages. The first step is data preparation, called data preprocessing, transforming the data and making it suitable for models. All data in this study is numerical (e.g. integer, float, etc.), and there is no missing data or data with a value of 0 (zero). The second stage consists of model selection, and in the third stage, the model is trained/developed and the first-order parameters that affect the predictions are determined. The quantiles of the micro-parameters and the UCS values are presented in Table 1 and the UCS values range from 17.8 to 111 MPa, presenting different rock types.

Table 1. Quantities of micro-parameters and estimated UCS parameter.

Parameter	Ave	Std	Min	%25	%50	%75	Max
N (-)	9.92	1.03	8.00	9.00	10.00	11.00	12.00
Y (GPa)	11.99	2.45	9.00	10.00	12.00	14.00	17.00
ϕ (°)	2.48	2.55	1.00	1.00	1.00	5.00	15.00
P (-)	0.43	0.05	0.30	0.40	0.40	0.50	0.50
t (MPa)	7.50	2.36	4.00	5.00	7.00	9.00	13.00
c (MPa)	77.69	29.23	25.00	59.00	74.00	90.00	180.00

UCS (MPa)	57.24	24.05	17.80	38.50	47.00	83.25	111.00
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*N: coordination number, Y: equivalent elastic modulus, ϕ : friction angle of particles, P: stiffness ratio, t: tensile strength of particles, c: cohesion of particles, and UCS: uniaxial compressive rock strength

LR (linear regression), DT (decision tree regression), and RF (random forest regression) methods were chosen respectively from the machine learning methods to predict the UCS values of the DEM model samples. LR is a well-known method for continuous and linear variables in the supervised machine learning technique. A linear curve is obtained by using one or more independent variables that accurately predict the value of the dependent variable (Figure 4a). The coefficient of the equation of this curve gives information about the reliability of the prediction. Since it uses a formulation that is relatively more practical to interpret, it is mostly preferred in statistical studies in various fields.

The second method, DT, used in classification and regression problems, consists of tree-structured algorithms. Since the target variable in this study is continuous (numerical), the algorithms are called DT regression trees here. A dataset is divided into smaller subsets as forming decision and leaf nodes according to feature and target (Figure 4b). It is worth noting that since DT regression is not continuous like other regression models but is discrete, it can produce the same results for the targeted predictions in a certain range.

The third method of the study, RF, is a regression method based on the principle of generating a random forest using more than one DT algorithm (Figure 4c). In other words, the average value of all DT predictions gives the result of RF. Because it uses DT algorithms, it is discrete and therefore can also produce the same results for the targeted predictions in a certain interval that care must be taken.

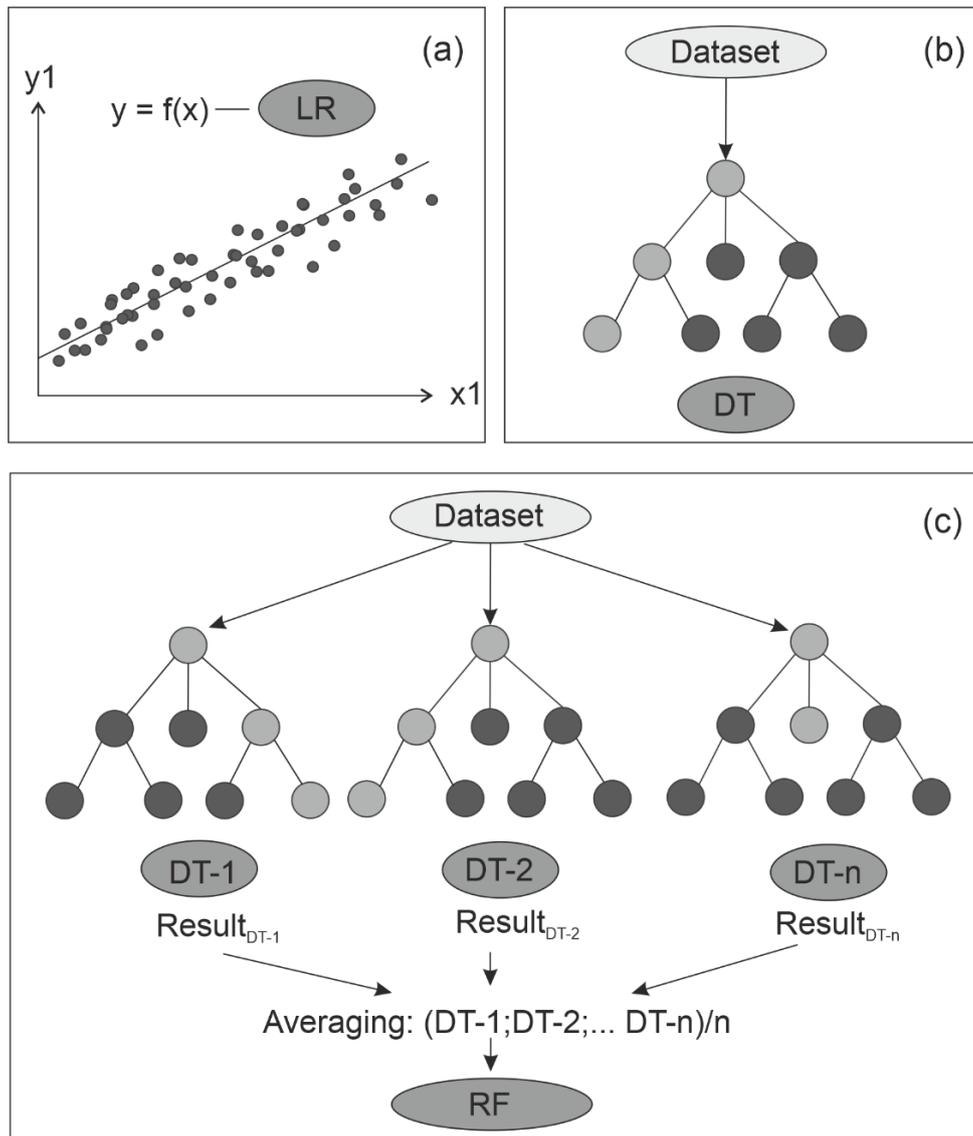


Figure 4. Configurations of the used machine learning methods a) LR (linear regression) b) DT (decision tree regression) and c) RF (random forest regression).

The coefficient of determination (R^2), mean squared error (MSE), mean absolute error (MAE), and root mean squared error (RMSE) metrics were used to evaluate the performance of the methods presented above. R^2 is a statistical measure of how close the model result is to the regression line, and

it is specifically used in the LR method (Eq. 5). In other words, if the R^2 value is close to 1, the data is close to the linear line. R^2 is calculated such that;

$$R^2 = 1 - \frac{\sum(y_i - y_i')^2}{\sum(y_i - y_{io})^2} \quad (5)$$

where y_i , y_{io} , y_i' are the actual, mean, and predicted values, respectively.

The second metric, MSE, is the mean square error, which measures the average squared difference between the y_i' and the y_i values and is derived from Eq. 6.

$$MSE = \frac{1}{N} \sum_{i=1}^N (y_i - y_i')^2 \quad (6)$$

The lower the MSE value the more accurate the model is. In other words, a value close to zero represents better quality of the predictor (regression model). However, since errors are squared when using this metric, exaggerated results can be produced in case of large deviations in the data.

RMSE is a square root of value gathered from the MSE function, shown in Eq. 7. It is used when the MSE is too large to be compared. The RMSE value can range from 0 to ∞ .

$$RMSE = \sqrt{\frac{\sum_{i=1}^N (y_i - y_i')^2}{N}} \quad (7)$$

It indicates how dense the data is around the line that best fits the data.

As the last metric used here, MAE measures the absolute difference between the y_i' and y_i values. Similar to MSE, the closer MAE is to 0, the more accurate the model is. In particular, MAE values of less than 10% show that the prediction models have high accuracy. It is calculated from Eq. 8 and is one of the most preferred metrics besides RMSE in the evaluation of model performances in regression methods.

$$MAE = \frac{1}{N} \sum_{i=1}^N |y_i - y_i'| \quad (8)$$

3. RESULTS AND DISCUSSION

Three different machine learning methods (LR, DT, and RF) described above were applied to estimate the UCS values of rocks obtained from 3D-DEM numerical models and the performances of the methods were evaluated according to R^2 , MSE, RMSE, and MAE metrics (Table 2). The results showed that the highest performance estimation was obtained from the LR method for all metrics. Especially based on the MSE results, the LR method provides better estimation/prediction than that of other methods. However, considering the relationship between the actual and predicted UCS values, regardless of the metrics, it is observed that all three methods' results are close to each other (Figure 5).

Table 2. Performance of the machine learning methods in UCS prediction according to the R^2 , MSE, RMSE, and MAE metrics.

Method	R^2	MSE	RMSE	MAE
LR	0.981	8.487	2.913	2.289
KA	0.895	41.221	6.420	5.398
RO	0.849	80.844	8.991	6.655

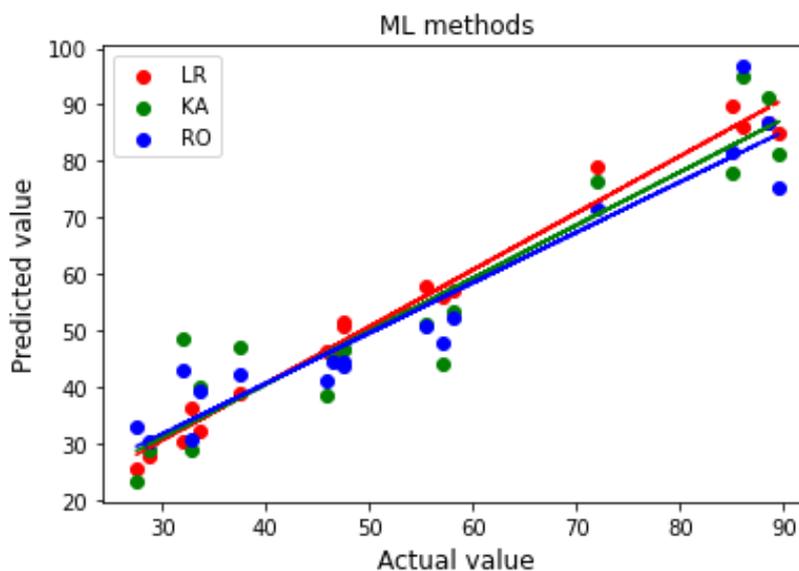


Figure 5. The relationship between the actual and estimated UCS values according to the LR, DT, and RF methods.

Doğan and Doğan [32] pointed out that since the R^2 metric estimates the combined distribution against the individual distributions of the observed and predicted variables, a model with systematically over- or under-estimates can produce R^2 values close to 1, even if all of the predicted values are incorrect. Therefore, three more metrics (MSE, RMSE, MAE) were considered in this study, since it is not sufficient to test a model's performance only with the R^2 value. Furthermore, it is highlighted in the literature that the mean error can produce misleading results in the performance evaluations of the methods in which the RMSE is considered [33]. It is noted that because the criteria based on the sum of squares of error are generally considered uncertain indicators, such as mean deviation, mean error, and mean variability, it can cause misinterpretations of the predictions [32]. Although it is suggested that MAE is generally a better criterion for such interpretations [33], one can

clearly realize that the use of these metrics strongly depends on the content, property, and usage area of the data.

Besides the comparison of the performance of machine learning methods in estimating the numerical UCS value, the most effective micro-parameters on this estimation were also determined. For this purpose, the feature/parameter selection process was applied to the dataset. In fact, this process is generally used in studies where too many variables are taken for estimation/prediction, and a faster and less complex model is created by eliminating the variables that have very little influence on the results. Because of the few numbers of parameters used in this study, there was no need to eliminate any variable (parameter). The UCS prediction was done by using all 6 micro-parameters.

Therefore here, the feature selection methodology was applied to reveal which micro-parameters play the most effective role in the prediction of the UCS value. For this purpose, a criterion called mutual information (MI), which measures the non-linear relation between random variables in probability and information theories, was used [34, 35]. It is the measure of how much knowledge one can acquire of a significant variable by knowing the value of another variable.

For two discrete variables x and y whose joint probability distribution is $P(x,y)$, the mutual information between them $MI(X;Y)$ is calculated such that;

$$MI(X; Y) = \sum_{x \in X} \sum_{y \in Y} p(x,y) \log\left(\frac{p(x,y)}{p(x)p(y)}\right) \quad (9)$$

MI ranges from 0 to 1. MI values that are close to 1 indicate relatively more effective parameters over the estimated/predicted feature (parameter) (Figure 6). As expected, MI results show that Y (equivalent elastic modulus), t (micro-tensile strength), and c (micro-cohesion) parameters play a more effective role on the UCS value than the others.

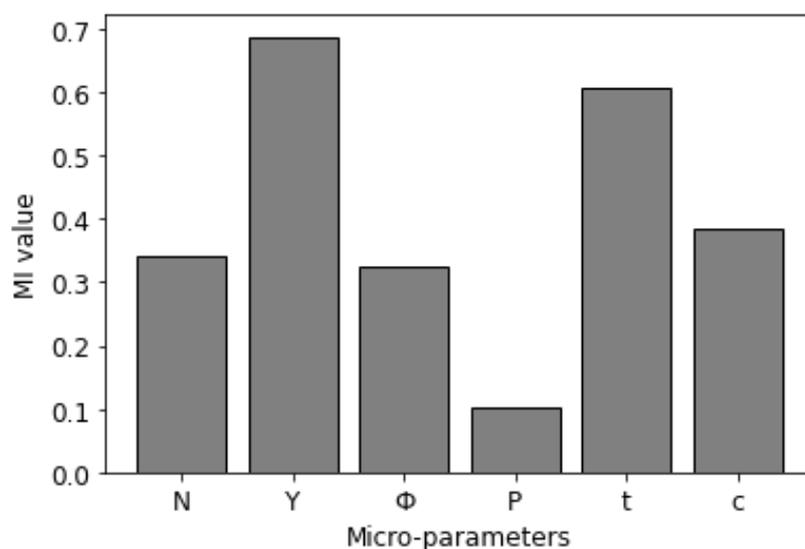


Figure 6. The most effective parameters in UCS prediction according to MI evaluation.

Although the metric results show that the applied machine learning methods produce good performances as well as predictions close to each other, the highest performance is obtained from the LR method. For this reason, the LR method was applied to the DEM model samples by assigning values for 6 micro-parameters and then the UCS value was predicted for validation. For instance, for the values of $N=9$, $Y=12$ GPa, $\varphi=1^\circ$, $P=0.4$, $t=6$ MPa, and $c=60$ MPa, the LR method gives the UCS value as 32.1 MPa, close to the calculated one. In general, this process took approximately about 36 minutes with a 3-core processor speed, whereas the estimation of the UCS value with the LR method took only a few seconds after running the script. Therefore, machine learning approaches can be used as reliable and practical tools in the calibration problems of particle-based DEM models that were also pointed out by Fathipour-Azar [29].

In the calibration of the numerical UCS value according to the real UCS value of a rock, the method suggested here provides extremely fast information in which values or at least ranges of the parameters should be selected before the simulation starts. This insight provides the user significant amount of time, especially in engineering applications where the high model resolution needs to be configured.

4. CONCLUSIONS

DEM-based numerical models provide important information for predicting the failure and deformation behaviors of rocks that host engineering structures. The reliability of this information is precisely based on the accuracy of the model generated. Therefore, the calibration process is critical to

implicitly represent the mechanical characteristics of real rock. This process sometimes takes an extremely long time, depending on the model resolution as well as the experience of the user.

In this study, the UCS values of 3D-DEM models calibrated with 6 micro-parameters were predicted by using machine learning methods, which became widely used in the field of rock mechanics recently. In the present research, LR, DT, and RF methods were tested in terms of their robustness, and the highest estimation performance for R^2 , MSE, RMSE, and MAE metrics was obtained from the LR method. Furthermore, the most effective parameters on the UCS value were determined as Y , c , and t micro-parameters with the feature selection methodology. The results show that machine learning methods can be used effectively in shortening and facilitating the calibration time of a 3D numerical DEM model and producing reliable results for the calibration process of micro-parameters of the model domain.

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The author declares that there is no conflict of interest.

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