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Predicting the Crack Stress Thresholds of the Intact Granitic Rocks by machine learning and multivariate analysis techniques

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Abstract

This research aims to significantly advance the understanding of crack stress thresholds in rocks by utilizing intelligent and statistical methodologies applied to a comprehensive database of granitic rocks. The database includes essential mechanical parameters, such as crack initiation stress and crack damage stress, as outputs, and unconfined compressive stress, Young's modulus, and Poisson's ratio as inputs. The study employs multivariate regression analysis (MRA), Decision tree (DT), and artificial neural network (ANN) techniques to analyze the data. To assess and compare the performance of these models, various metrics are used, including root-mean-square error (RMSE), mean absolute error (MAE), coefficient of determination (R^2), mean absolute percent error (MAPE) and the a20-index. The findings reveal that the ANN method surpasses MRA-based and decision tree regression-based approaches in accurately predicting the output parameters. The ANN model demonstrates outstanding predictive performance for σ_{ci}, achieving an R^2=0.934, RMSE=5.965, MAE=4.79, MAPE=5.3% and VAF=93.34%. Similarly, the model excels in predicting σ_{cd} with an R^2=0.985, RMSE=4.676, MAE=3.785, MAPE=2.3%, VAF=98.4%, Additionally, sensitivity analysis identifies unconfined Compressive stress (UCS) as the most critical factor in predicting crack initiation stress (σ_{ci}) and crack damage stress (σ_{cd}). The findings suggest that the ANN model is more effective in predicting σ_{ci} and σ_{cd} of rocks compared to other methods.

Keywords

Uniaxial Compressive Strength, Multivariate regression analysis, Artificial neural network, Decision tree, Crack stress thresholds

1 Introduction

A comprehensive understanding of the spatial distribution of various cracks within rock masses is crucial not only for advancing the fundamental study of rock failure mechanisms but also as an essential tool for assessing geotechnical risks. Previous research extensively examined the formation and distribution of crack patterns by analyzing the failure characteristics of different crack types. Scholars identified distinct parameters associated with various crack types using specific tests, such as the uniaxial compression test (Vásárhelyi, 2000), the Brazilian splitting test (Chang et al., 2020), and the three-point bend fracture test (Rozière et al., 2007). These tests provided valuable insights into the behavior and development of cracks under different stress conditions.

The essential characteristic stress thresholds in the failure process are the crack initiation stress (σ_{ci}) and the crack damage stress (σ_{cd}). While crack initiation denotes the beginning of micro-fracturing, crack damage denotes the beginning of crack coalescence and dilatation deformation (volumetric strain).

There is a limited amount of research focused on the relationship between rock properties and crack stress thresholds. However, it is suggested that the crack initiation stress (σ_{ci}) is a reliable indicator for predicting both crack initiation and damage stress levels. Despite this, no significant correlations have been found between crack stress thresholds and the stiffness properties of rocks, highlighting a gap in understanding these interactions (Pepe et al., 2018); Although, Narimani et al. (2023 and 2024a) introduced a new approach to calculate the elastic stiffness parameters and Poisson's ratio of granitic rocks from the crack closure phase up to the failure stage. This method provides a more detailed understanding of the variations in stiffness and Poisson's ratio throughout the rock's loading process. Many studies exist in the literature exploring the statistical relationships among the physical, mechanical, and ultrasonic properties of rocks. These studies aim to develop nondestructive testing solutions that facilitate quick and accurate predictions of specific parameters (Zhu et al. 2010; Kahraman 2001; Mutaz et al. 2021).

Leveraging artificial intelligence (AI) and machine learning (ML) has opened new possibilities in the field of rock mechanics, particularly in predicting critical rock mechanical properties and thresholds related to rock damage. Despite the progress, using these advanced algorithms to estimate rock mechanical parameters from fundamental physical and ultrasonic rock properties is still in an emerging phase. The potential of AI and ML in this area could revolutionize traditional approaches, allowing for more accurate and efficient analyses compared to conventional methods. In recent research, Narimani (2024b) applied various ML models to predict two key rock properties: unconfined compressive strength (UCS) and Young's modulus. By training these models on comprehensive laboratory data—including density, P-wave velocity, shear strength, and tensile strength measurements of granite—Narimani demonstrated that AI-driven techniques could offer accurate estimations of these properties. Shahani et al. (2022) employed ANFIS, artificial neural network (ANN), and MVLR methods to predict UCS weak rocks. Their study demonstrated the potential of these methods for accurately predicting rock strength properties. Several researchers and practitioners in geotechnical engineering have emphasized the potential of machine learning (ML) methods, such as decision trees (DTs) and artificial neural networks (ANNs) to predict key rock mechanical parameters. These ML techniques are being increasingly applied for enhanced accuracy in forecasting complex rock behavior, thereby aiding in more reliable geotechnical assessments and engineering decisions (Sharma, 2017; Wei et al. 2023).

This paper seeks to evaluate the effectiveness of machine learning (ML) techniques in predicting crack stress thresholds by leveraging fundamental rock mechanical properties. The study is built on data obtained from laboratory tests conducted on granitic rocks, specifically drawing on the experimental work of Nicksiar (2012). The primary goal is to investigate how well ML models can estimate the critical stress levels at which cracks initiate and propagate, using input features such as uniaxial compressive strength, Young's modulus, and Poisson's ratio. By comparing ML predictions with empirical data, the study aims to determine whether machine learning can serve as a reliable method for forecasting crack behavior in rocks, thus offering a more advanced approach for geotechnical applications.

2 Materials and Data analysis

When brittle rocks are exposed to uniaxial compression, their stress–strain behavior can be broken down into five distinct phases, as outlined by Eberhardt et al. (1999). The process begins with **Stage I**, where existing microcracks and flaws within the rock close under increasing stress. In **Stage II**, the rock undergoes linear-elastic deformation, where the material deforms without permanent damage. As the load increases further, **Stage III** occurs, characterized by the formation and stable propagation of new cracks. During **Stage IV**, these newly formed cracks grow in an unstable manner, leading to rapid

damage accumulation. Finally, the rock reaches **Stage V**, where ultimate failure occurs, followed by a post-failure phase, indicating the complete breakdown of the material structure (Fig.1).

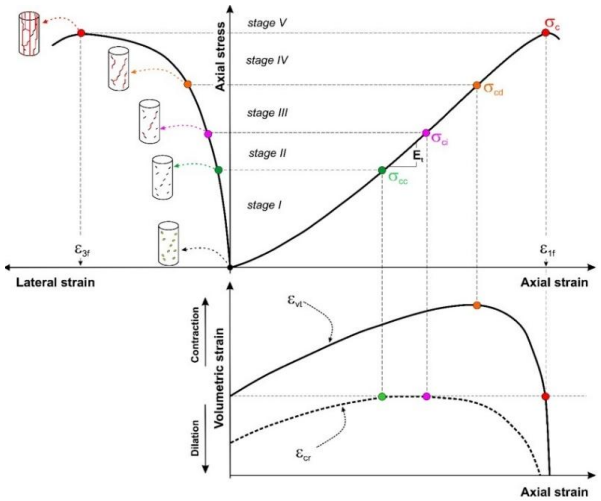


Fig 1. Stress–strain diagrams depicting the behavior of intact rock under uniaxial compression, highlighting the key stages of progressive brittle damage (modified from Eberhardt et al. 1999).

This research explores various foundational machine learning methods, including multi-linear regression, multi-non-linear regression, and step-wise regression models, as well as Artificial Neural Networks (ANN) and Decision Trees (DT), all implemented using MATLAB (2019). The investigation centers on experimental data from extensive laboratory testing on granitic rock specimens, largely derived from Nicksiar's (2012) research. A dataset of 107 granitic rock samples was processed, with an 80% subset allocated for model training and the remaining 20% reserved for testing. Key performance metrics were calculated to assess each model's accuracy in predicting stress thresholds.

The primary research aim is to forecast two specific stress points in the granitic rocks: initial crack stress and damage crack stress. The models leverage fundamental material properties, including Uniaxial Compressive Strength (UCS), Elastic Modulus (E), and Poisson's Ratio, to make predictions regarding these stress levels. The research approach is visually detailed in a flowchart (see Figure 2), which lays out the methodology comprehensively and aligns each step with the study's objectives.

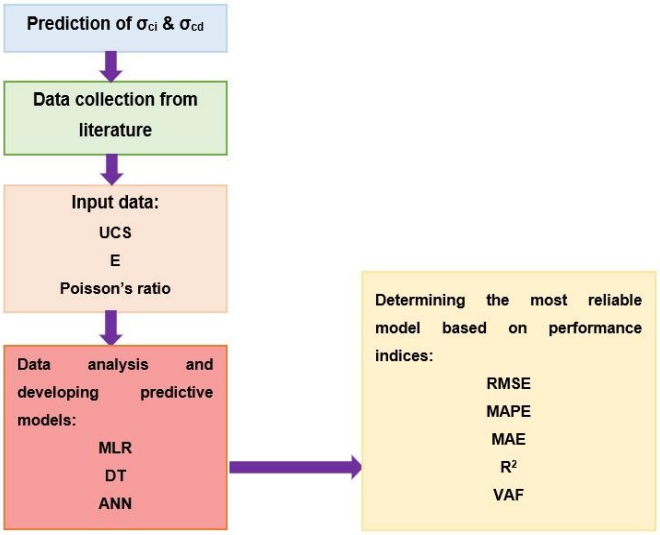


Fig. 2 Flowchart of the proposed research

The study examines the relationships between various parameters, including UCS, E, Poisson's ratio, crack initiation stress, and crack damage stress, using both machine learning and statistical analysis. UCS, E, and Poisson's ratio are utilized as input variables to predict crack initiation and damage stresses. A correlation matrix is employed to analyze the variance and covariance in the regression model, helping to understand how the variables interact. Figures 3 illustrate the pairwise correlations among the input and output variables. These visualizations reveal positive, negative, or neutral relationships, highlighting how different variables influence one another. Stronger correlations indicate a greater impact on model accuracy and efficiency, enhancing the understanding of the inputs' effects on the outputs.

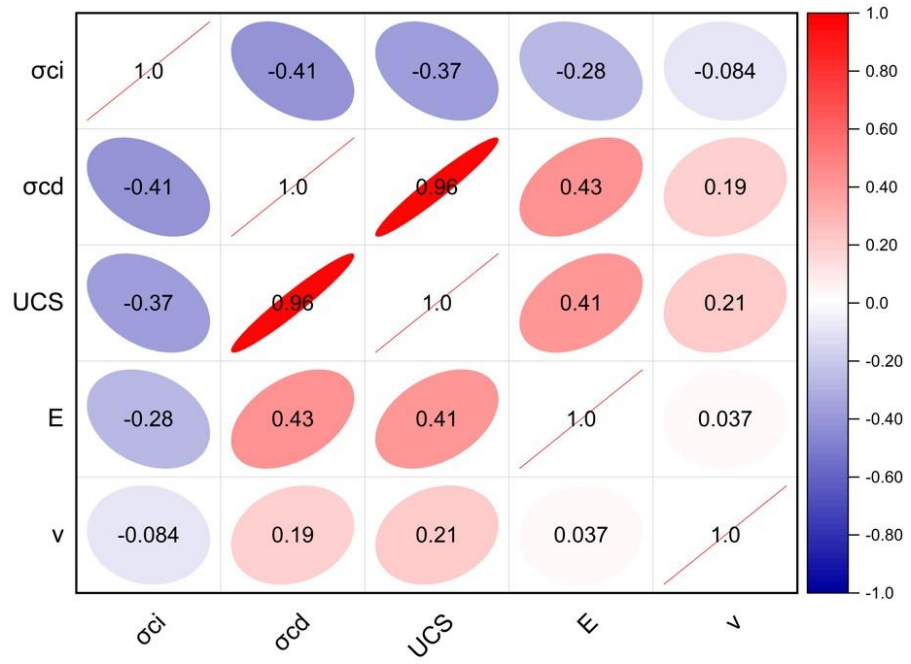


Fig. 3 Correlation matrix of inputs and outputs

3 Results

3.1 Multivariate Linear Regression (MLR)

Multivariate Linear Regression (MLR) is an advanced extension of linear regression that uses empirical observations to derive a mathematical relationship between a dependent variable y and multiple independent variables x, along with an error term ε. The primary aim is to explore how the dependent variable is influenced by the predictors and compare MLR's predictive capabilities with alternative machine learning methods. For instance, an MLR model involving two predictors can be expressed as follows (Tiryaki, 2008):

$$Y = \beta_0 + \beta_1 \times X_1 + \beta_2 \times X_2 + \varepsilon \quad (1)$$

where β_0 = intercept term; β_n = coefficient term; ε = noise term; X_n = independent variables. Finally, two multiple linear regression equations were extracted for predicting σ_{ci} and σ_{cd}:

$$\sigma_{ci}\ (\text{MPa}) = -32.119 + 0.423*UCS + 0.506*E + 10.729*\nu \quad (2)$$

$$\sigma_{cd}\ (\text{MPa}) = -10.938 + 0.783*UCS + 0.265*E - 3.321*\nu \quad (3)$$

3.2 Decision Tree (DT)

Decision Trees (DTs) are versatile tools used for classification and regression tasks. These non-parametric supervised learning models operate by sequentially splitting data into subsets based on specific decision criteria, forming a tree-like structure of "if-then-else" rules. A well-constructed DT aligns closely with actual data, improving prediction accuracy as its depth increases. DTs are effective for analyzing both small and large datasets and are particularly useful for solving prediction problems. They offer a straightforward approach to understanding relationships between variables and identifying the most influential ones. By visualizing decisions as branches and outcomes as nodes, decision trees provide a clear breakdown of all possible scenarios and their implications. This structured method enables thorough exploration of alternatives, ensuring informed decision-making while mapping potential outcomes comprehensively. A simple schematic is shown in Figure 4.

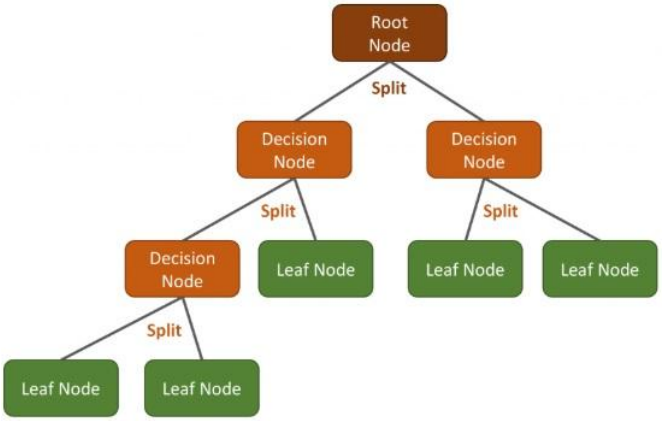


Fig. 4 Decision Tree schematic showing root node, decision nodes and leaf nodes.

3.3 Neural Network Analysis

An Artificial Neural Network (ANN) is a machine learning approach inspired by the structure and function of biological neural networks. It aims to establish direct relationships between input and output variables without relying on predefined assumptions. ANNs comprise three core elements: the transfer function, network architecture, and learning rule, which collectively address complex statistical problems (Figure 5). In this research, ANN computations were implemented using MATLAB's toolbox. Among various architectures, the Multilayer Perceptron (MLP) is one of the most widely used models in engineering. The MLP operates as a supervised learning system, utilizing backpropagation to adjust connection weights iteratively. This process enhances model accuracy by minimizing training errors and improving prediction performance. A three-layered MLP model structure was employed. For optimizing training, the Levenberg-Marquardt algorithm proved effective, particularly in scenarios requiring error minimization, such as with mean squared error or normalized squared error. This study assessed the ANN model's effectiveness by analyzing training and validation error metrics.

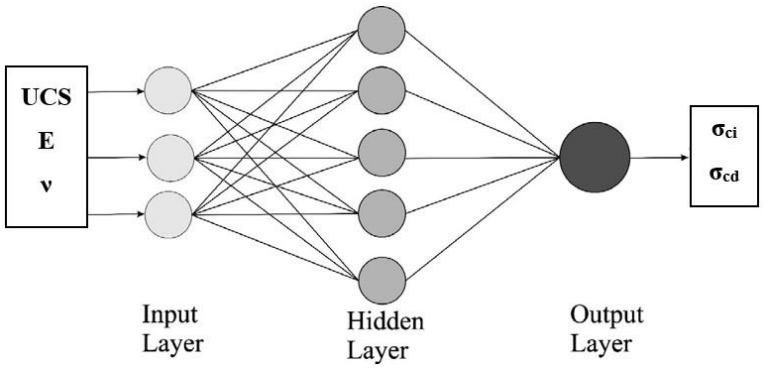


Fig. 5 The structure of neural network.

3.4 Model Evaluation

The dataset collected consisted of 107 data points related to the testing and evaluation of geomechanical properties, serving as the core foundation for validating the proposed methodology. The prediction accuracy for σ_{ci} and σ_{cd} was evaluated using four standard statistical metrics: root mean square error (RMSE), mean absolute error (MAE), mean absolute percentage error (MAPE), and variance accounted for (VAF). These performance metrics are defined by Equations (4) to (7).

$$\text{RMSE}=\sqrt{\frac{\sum_{i=1}^{n}(pi-qi)^2}{n}} \quad (4)$$

$$\text{MAPE}=\frac{1}{n}\sum_{i=1}^{n}\left|\frac{qi-pi}{qi}\right|\times 100 \quad (5)$$

$$\text{MAE}=\frac{\sum_{i=1}^{n}|pi-qi|}{\text{n}} \quad (6)$$

$$\text{VAF} = [1-\frac{var(pi-qi)}{var(pi)}]\times 100 \quad (7)$$

In this context, 'n' represents the total experiment count, 'pi' and 'qi' denote the projected and expected findings for the ith experiment respectively. The ideal scenario is achieved when RMSE = 0, MAE = 0, MAPE = 0, VAF = 100. Tables 1 and 2 present the rankings, offering a numerical evaluation of σ_{ci} and σ_{cd}. The results reveal that the MLR model, with a total score of 5, performed the poorest in predicting σ_{ci} and σ_{cd}, consistently trailing behind the other models. In contrast, the DT model showed improved accuracy, securing the second position overall, while the ANN model emerged as the best-performing method, delivering the most accurate predictions.

Table 1 Performance comparison of σ_{ci} for all the models.

Model	R^2	Score	RSME	Score	MAE	Score	MAPE	Score	VAF (%)	Score	Rank
MLR	0.782	1	10.660	1	8.540	1	0.093	1	78.72	1	5
DT	0.853	2	9.002	2	7.346	2	0.082	2	84.84	2	10
ANN	0.934	3	5.965	3	4.790	3	0.053	3	93.34	3	15

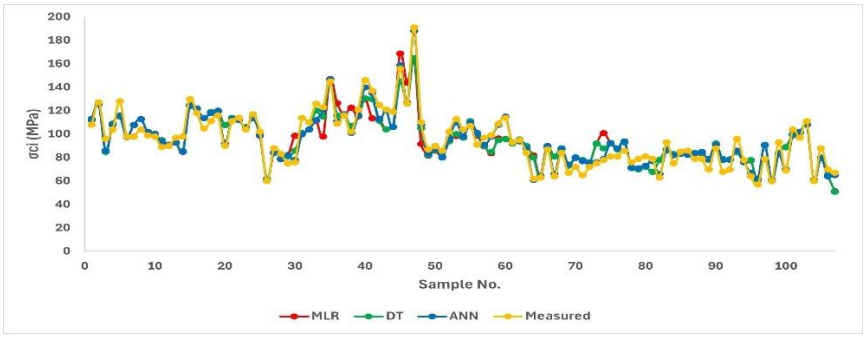
Table 2 Performance comparison of σ_{cd} for all the models.

Model	R^2	Score	RSME	Score	MAE	Score	MAPE	Score	VAF (%)	Score	Rank
MLR	0.924	1	10.129	1	8.078	1	0.049	1	92.45	1	5
DT	0.957	2	7.813	2	6.388	2	0.039	2	95.52	2	10
ANN	0.985	3	4.676	3	3.785	3	0.023	3	98.40	3	15

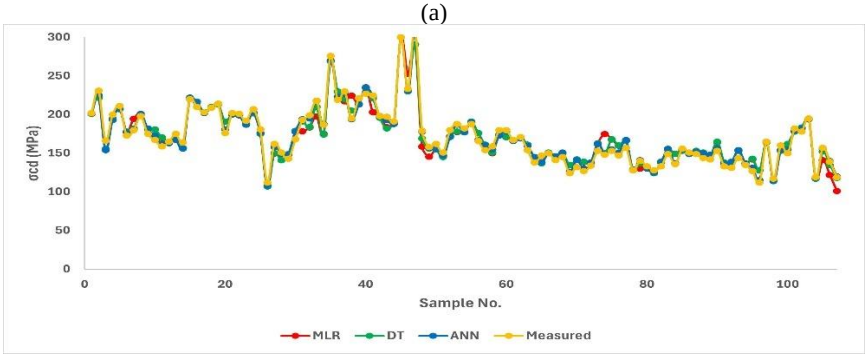
Drawing from the findings presented in Table 1 and Table 2, it becomes clear that among the various empirical and artificial intelligence approaches, the Artificial Neural Network (ANN) model emerges as the most effective and reliable method for predicting the parameters σ_{ci} and σ_{cd}. To visualize and compare the distinct performance levels of the models, graphs are provided in Figures 6 and 7. These graphs include compressive prediction curves and regression diagrams, highlighting how empirical and artificial intelligence techniques perform in modeling the data. Examining Figure 6, the prediction curves of σ_{ci} and σ_{cd} generated by all three models demonstrate a consistent alignment with the original data. However, the ANN model distinctly outshines the other methods, showcasing superior accuracy and reliability. Moving to Figure 7, the regression diagrams reveal a clear performance hierarchy. The ANN model achieves the highest coefficient of determination (R^2), recording values of 0.934 for σ_{ci} and 0.985 for σ_{cd}. This exceptional accuracy highlights ANN's robustness in modeling complex data. Among the remaining models, the Decision Tree (DT) shows relatively good performance, surpassing the Multiple Linear Regression (MLR) model in predictive capability.

3.5 Sensitivity Analysis

Sensitivity analysis identifies the influence of input variables in predictive models using linear and nonlinear techniques. The Cosine Amplitude Method (CAM) recently assessed the sensitivity of UCS, E, and ν, with CAM values close to 1 indicating high sensitivity. Results show UCS (0.98853) strongly impacts σ_{ci} prediction, while E (0.98068) dominates σ_{cd} prediction (Figure 8).

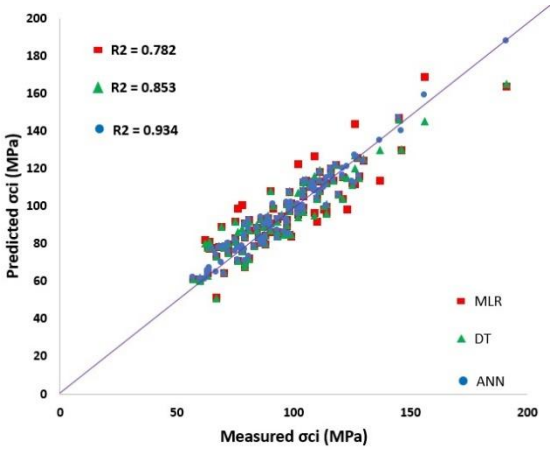


(a)

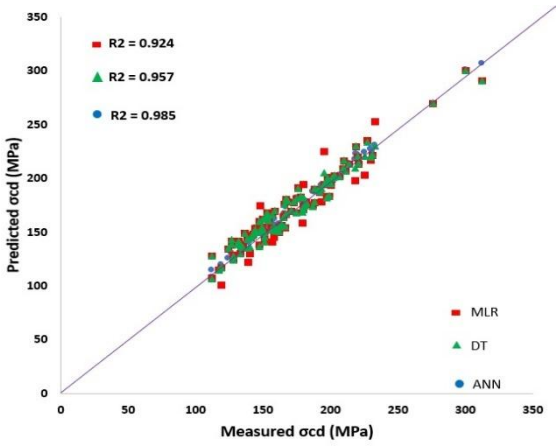


(b)

Fig. 6 Comparison of the (a) σ_{ci} and (b) σ_{cd} results predicted by the MLR, DT and ANN models with the actual ones.

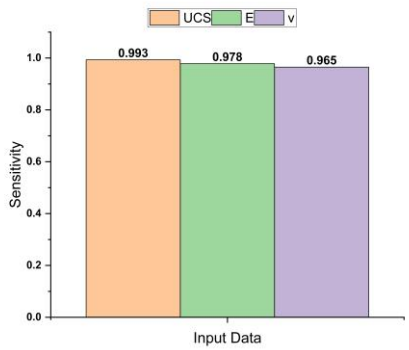


(a)

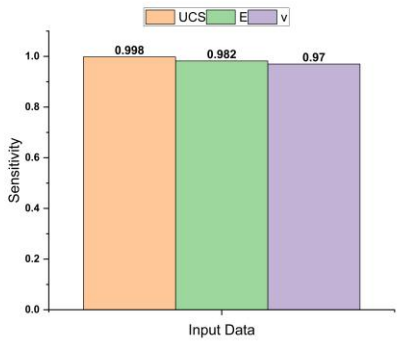


(b)

Fig. 7 Measured and predicted (a) σ_{ci} and (b) σ_{cd} using MLR, DT and ANN model.



(a)



(b)

Fig. 8 The impact of input variables on model outcomes, (a) σ_{ci} and (b) σ_{cd}

4 Conclusions

This research focused on the development of advanced intelligent predictive models specifically designed to estimate the crack stress thresholds (σ_{ci} and σ_{cd}) in granitic rocks. To achieve this, a robust and detailed database was compiled, encompassing the mechanical properties of various types of granitic rocks through an extensive review of existing literature. Key parameters such as UCS, E and ν were identified and used as input variables in the modeling process. A range of machine learning (ML) algorithms, including Artificial Neural Networks (ANN), Decision Trees (DT), and the more traditional Multiple Linear Regression (MLR) techniques, were employed to construct the predictive models. The comparative analysis demonstrated that ANN significantly outperformed both DT and MLR, delivering superior accuracy and reliability in predicting the crack stress thresholds. This highlights the ANN model's ability to reduce uncertainties in rock engineering applications. The utilization of soft-computing models, such as ANN, brings several advantages, including computational efficiency and the elimination of the need for complex instrumentation. However, developing and validating these models often requires extensive datasets, a challenge exacerbated by the limited availability of geotechnical data. Despite this limitation, the findings of this study offer considerable potential to enhance geotechnical engineering practices.

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