

Results in Geophysical Sciences

Prediction of uniaxial compressive strength and modulus of elasticity for Travertine samples using an explainable artificial intelligence

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ABSTRACT

The durability of rocks is a substantial rock property that has to be considered for designing geotechnical structures. Uniaxial compressive strength (UCS) and Young's modulus (E) are key indexes for measuring rocks' durability. Several types of artificial intelligence (AI) methods have been used for modeling these key indexes; however, surprisingly, no explainable AI (XAI) has been considered for their model developments. An XAI is a model whose assessment is not a black box, and humans could understand its problem solution approach. This study has filled this gap and presented SHAP (Shapley Additive Explanations) as one of the most recent XAI methods for modeling UCS, and E. SHAP value could successfully illustrate intercorrelations between rock properties (porosity, point load index, P-wave velocity, and Schmidt hammer rebound number) and their representative UCS and E for each individual record and also together as variables. Results indicated that P-wave velocity has the highest importance for UCS and E prediction. eXtreme gradient boosting (XGBoost) was used as a solid predictive AI system for UCS and E estimation. Outcomes ($R^2 > 0.99$) confirmed the high accuracy of the SHAP-XGBoost model comparing with other typical AI models (Random Forest and Support Vector Regression). These results indicated XAI could be considered for illustrating complicated relationships within rock mechanics and energy-resource developments.

1. Introduction

Travertine is one of the main rocks for the construction industry. Its durability as an essential property has been used to determine its different applications for centuries. In rock engineering, uniaxial compressive strength (UCS) and the young' modulus of elasticity (E) are two main factors that have been widely considered to assess travertine and other rocks' durability. These factors have been implemented to classify rocks based on their elastic deformation. The elastic deformation is a key feature to quantify stress fields and failure points of rocks. Determination of these properties would be essential for developing various fossil fuel resources, mining, dams, and many other facilities ((Anon, 1978), (Demirdag et al., 2010; Dehghan et al., 2010; Armaghani et al., 2015; Hakan and Kanik, 2012; D.J. Armaghani et al., 2016; Török and Vásárhelyi, 2010)).

American standards for testing materials (ASTM E111–17) are typical methods for measuring the E (D.J. Armaghani et al., 2016; Jamshidi et al., 2016; Sousa, 2014). On the other hand, the International

Society for Rock Mechanics (ISRM) has been developed a standard test for the UCS determination. However, these direct measurements are expensive and time-consuming. In addition, providing adequate representative core samples to evaluate possible measurement errors would be difficult. Since UCS and E depend on the rocks' structure and their characteristics, several different statistical and computational models have been developed to predict them based on various rock properties (porosity (n), water content and absorption, mineralogy) and rock indexes (point load strength index ($I_p(50)$), P-wave velocity (V_p), Schmidt hammer rebound number (R_n)) for filling this gap (Table 1). These artificial intelligence models as black boxes are mainly successful in UCS and E predictions. Still, they could not provide any insight into relationships among rock properties and their durability indexes (UCS and E) (Matin et al., 2018; Salehin et al., 2020; Ozbek et al., 2013; Moussas and Diamantis, 2021). Few studies considered variable importance measurements, and typically, the main target was just gaining a high coefficient of determination (R^2) for the generated predictive models. Constructing explainable AI (XAI) models could potentially overcome

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Table 1

Various machine learning methods were used for the UCS and E prediction.

Input	Output	Model	R ²	References
n, w, γ	UCS	GEP	0.99	(Ozbek et al., 2013)
n, R _n , Vp, Is(50)	UCS	GP	0.84	(Fang et al., 2021)
n, R _n , Vp, Is(50)	E	GMDH	0.96	(Armaghani et al., 2020)
R _n , Vp, Is(50)	UCS	SFS-ANFIS	0.98	(Jing et al., 2020)
n, w, Vp, Is(50), RC, d	UCS	ICA-GFFN	0.98	(Asheghi et al., 2019)
Vp, d, SDI	UCS	ANFIS	0.98	(Sharma et al., 2017)
R _n , Vp, DD	UCS	GMDH	0.86	(Li et al., 2020)
n, R _n , Vp, Is(50)	UCS	GPR	1.00	(Mahmoodzadeh et al., 2021)
Gamma ray, Neutron porosity, Bulk density, Compressional time, Shear time	E	ANN	0.96	(Elkhatatny et al., 2019)
R _n , Vp, L	UCS	LS-SVM	0.87	(Çelik, 2019)
Vp, d, Qt	UCS	ANN-PSO	0.91	(Ebdali et al., 2020)

n porosity, w water absorption, γ dry unit weight, R_n Schmidt Hammer rebound number, Vp p-wave velocity, Is(50) point load strength index, RC rock class, d density, SDI slake durability index, DD dry density, L cubic sample sizes, Qt Brazilian tensile strength, GEP genetic expression programming, GP genetic programming, GMDH group method of data handling, SFS stochastic fractal search, ANFIS adaptive neuro-fuzzy inference system, ICA imperialism competitive algorithm, GFFN generalized feedforward neural network, GPR gaussian process regression, ANN artificial neural network, LS-SVM least square support vector machines, PSO particle swarm optimization.

these drawbacks.

In contrast with a “black box” model, in which even its designer cannot describe its specific decisions, an XAI can translate its outcome toward human-understandable. XAI models are significantly taking roles in our daily activities. SHAP (Shapley Additive Explanations) is one of the most recently developed XAI methods to analyze model interpretability. SHAP can illustrate the contribution (negative or positive) of each variable (all records of each variable together) and each record (each individual record of a variable) on the target and increase the prediction model transparency. SHAP can be used for any tree-based model. Recently, various disciplines have been expanded the application of XAI models; however, they have yet to appear expressively in the structural and rock engineering literature (Lundberg and Lee, 2017; Chelgani, 2021; Aas et al., 2021; Park and Park, 2021).

This investigation aims to introduce SHAP as an XAI method for assessing relationships between various rock properties and their representative UCS and E through their predictions using eXtreme gradient boosting (XGBoost). As a newly developed tree-based model, XGBoost is extremely flexible, has parallel processing power, supports regularization, and handles missing data (Mo et al., 2019; Mangalathu et al., 2021; Mao et al., 2021). For the first time, this study is going to consider the SHAP-XGBoost combination for assessing a rock mechanic problem. Random forest (RF) and support vector regression (SVR) as typical machine learning (ML) methods, and Pearson correlation as a linear correlation assessment index were used for validation and comparison purposes. The outcomes of this investigation would be verified the potential of SHAP-XGBoost as a reliable and accurate XAI tool for modeling complicated relationships within rock mechanic and natural structure engineering disciplines.

2. Materials and methods

2.1. Database

For providing a representative dataset, ten-block Travertine samples

Table 2

The statistical description of the mechanical rock properties of the Travertine from Hajiabad mine, Iran.

Variables	Min	Max	Mean	Std
PLI (MPa)	2.26	4.01	3.17	0.42
Vp (km/s)	4.82	5.81	5.36	0.27
R _n	25.62	30.50	27.87	1.43
n	0.97	10.27	6.58	2.92
E (GPa)	3.05	11.45	5.36	1.99
UCS (MPa)	22.70	71.54	38.99	12.59

were prepared from the Hajiabad mine, Iran. Thirty sets of samples were obtained from these blocks, and different tests (I_s(50), n, V_p, and R_n) were conducted to determine their rock properties. All the rock property assessments were conducted based on the standard procedure, which was recommended by ASTM E111–17, ISRM (1985), and ISRM (1981) (Franklin, 1985). The statistical evaluations of sample properties were presented in Table 2.

2.2. SHapley additive exPlanations (SHAP)

Model interpretability is a key problem for ML approaches. SHapley Additive exPlanation (SHAP) is a method for interpreting ML models predictions using Shapley values (Wen et al., 2021) that was proposed by Lundberg and Lee (Lundberg and Lee, 2017). The Shapley value for each feature is the average of all feature permutations' marginal contributions, representing the impact of that feature on the generated output (Parsa et al., 2020; Chelgani et al., 2021). The SHAP explanation model ($g(z)$) is established as a linear addition of input features and can be formulated as follows:

$$f(\mathbf{x}) = g(\mathbf{z}') = \phi_0 + \sum_{i=1}^M \phi_i z'_i \quad (1)$$

where $\mathbf{z}'$ is the simplified input, M denotes the number of features, ϕ_0 is a constant value, and z'_i is a binary variable that represents i th feature is being observed or not (Mangalathu et al., 2021; Meng et al., 2021). Given a model f , Shapley values ϕ_i for each input feature can be computed as Eq. (2).

$$\phi_i = \sum_{S \in N \setminus \{i\}} \frac{|S|!(M - |S| - 1)!}{M!} [f(S \cup \{i\}) - f(S)] \quad (2)$$

where S is a set including non-zero indexes in $\mathbf{z}'$ and N represents the set of all input features (Parsa et al., 2020; Meng et al., 2021; Chehreh Chelgani et al., 2021).

2.3. Extreme gradient boosting (XGBoost)

Extreme Gradient Boosting (XGBoost) is a gradient boosting library that has been optimized for efficiency, flexibility, and portability. XGBoost was developed by Chen and Guestrin (Chen and Guestrin, 2016) in 2016. XGBoost is an extension to gradient boosted decision trees (Nasiri and Hasani, 2021), which provides a parallel tree boosting to efficiently solve classification and regression problems (Movsessian et al., 2021; Yang et al., 2021; Qiu et al., 2021). The Newton-Raphson method is the foundation of XGBoost. Instead of just computing and following the gradient, it employs the second-order derivative (Hessian) to better approximate the direction of the maximum descent and its step size. XGBoost enhances model generalization by applying a variety of regularization methods, such as L₁ regularization (Lasso) and L₂ regularization (Ridge) (Y. Zhou et al., 2019; Gómez-Ríos et al., 2017; Nasiri and Alavi, 2021).

Given an input feature vector $\mathbf{x} = [x_1, x_2, \dots, x_n]^T$, the estimated output of the model $\hat{y}$ can be computed as follows:

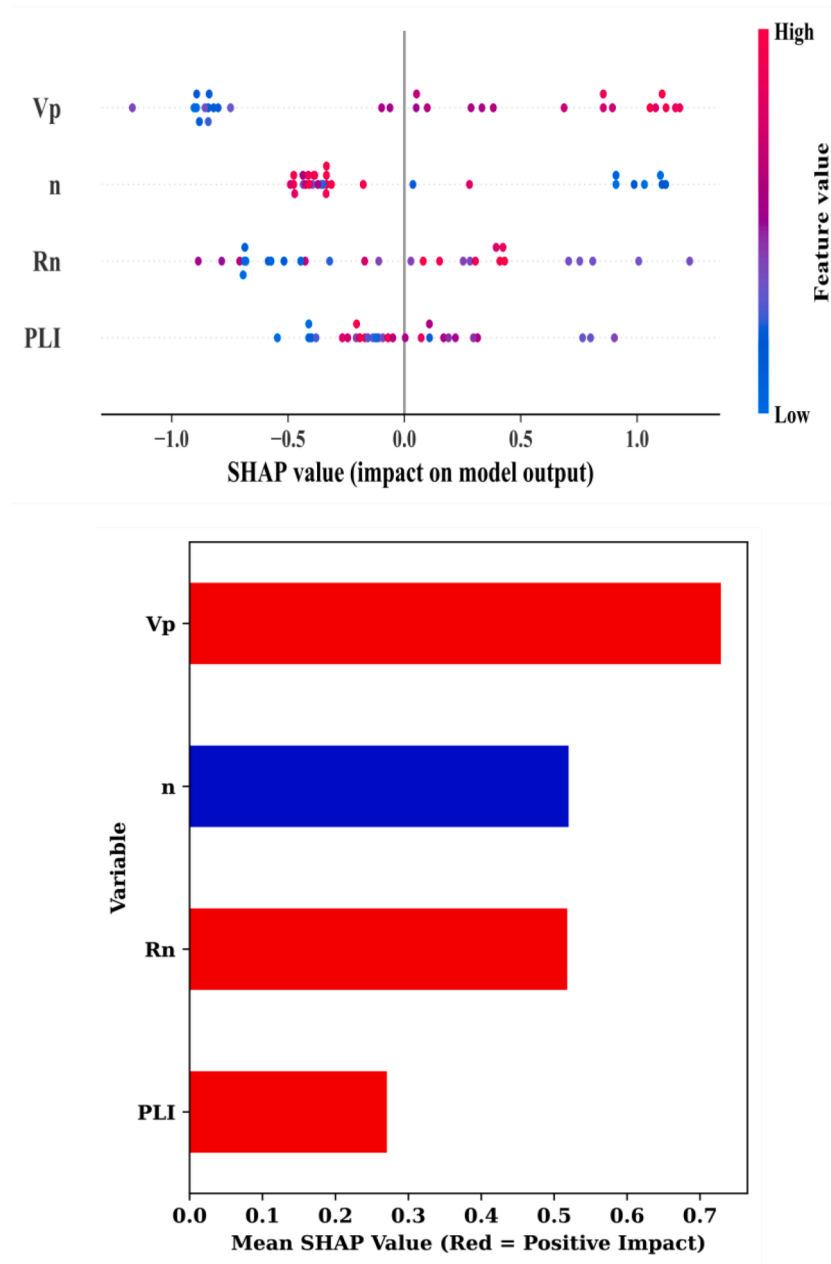


Fig. 1. SHAP assessment for exploring relationships between travertine properties with their representative young modulus.

$$\hat{y} = \sum_{k=1}^K f_k(\mathbf{x}), f_k \in \Gamma \quad (3)$$

where K denotes the number of weak learners, $f_k(\mathbf{x})$ is a prediction score, and Γ represents the hypothesis space of weak learners (Song et al., 2020; Zhang et al., 2021). Different sets of weak learners are trained by minimizing the objective function of Eq. (4) (Movsessian et al., 2021).

$$Obj(\theta) = L(\theta) + \Omega(\theta) \quad (4)$$

where $L(\cdot)$ is the loss function and $\Omega(\cdot)$ is the regularization function used to control the model's complexity and is computed as Eq. (5).

$$\Omega(\theta) = \gamma N + \frac{1}{2} \lambda \|w\|^2 \quad (5)$$

where γ and λ are parameters that regulate the penalty associated with the number of leaves N and the weight of each leaf, respectively (Jiang et al.,

2019; Osman et al., 2021; Wang et al., 2018).

2.4. Random forest

Random Forest (RF), which were developed by Breiman (Breiman, 2001), is a nonparametric ensemble method that gained tremendous success in several fields due to its ability to handle different forms of data (Wang et al., 2017; Tohry et al., 2020; J. Zhou et al., 2019; Hou et al., 2021; Srinivasan et al., 2020). As an ensemble method, RF is robust to outliers, produces an unbiased estimate of the generalization error, reduces overfitting, has versatility, can handle missing data, and has no statistical assumption (Gong et al., 2018; Oualloche et al., 2018; Trehan and Durlinsky, 2018). RF is a collection of tree predictors that are grown independently. So individual trees predictions are aggregated by averaging to produce a final prediction (Segal and Xiao, 2011; Schauburger and Groll, 2018; Kardani et al., 2021).

Formally, given an input feature vector $\mathbf{x} = [x_1, x_2, \dots, x_n]^T$, the RF

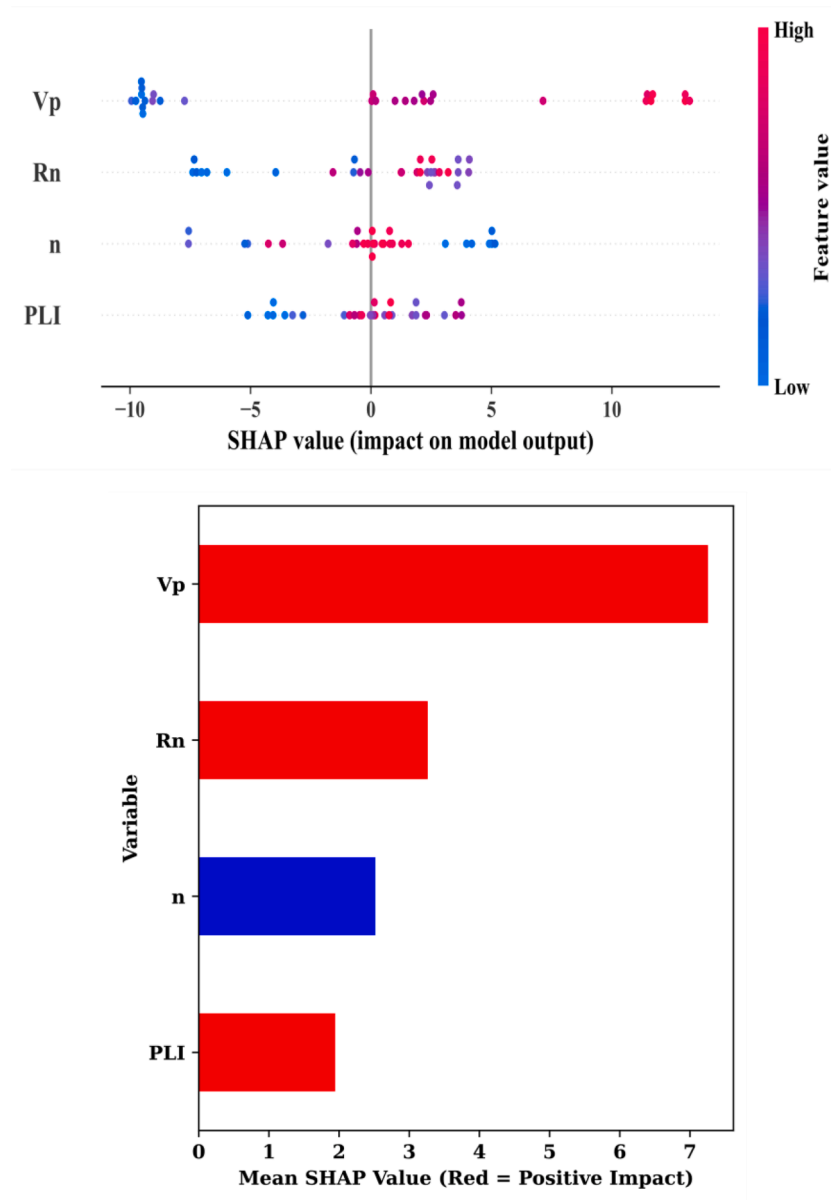


Fig. 2. SHAP assessment for exploring relationships between travertine properties with their representative UCS.

model's predicted output $\hat{\tau}(\mathbf{x})$ can be computed as follows:

$$\hat{\tau}(\mathbf{x}) = \frac{1}{B} \sum_{b=1}^B \hat{\tau}_b(\mathbf{x}) \quad (6)$$

where B denotes the number of trees and $\hat{\tau}_b(\mathbf{x})$ is the estimation generated by b th tree (Wager and Athey, 2018; Jafrasteh et al., 2018)

2.5. Support vector regression

Support Vector Regression (SVR) is a nonparametric statistical method proposed by Drucker (Drucker et al., 1997) and his colleagues in 1996. SVR is robust to outliers, has high generalization capability, and can learn nonlinear dependencies of the data, and its computational complexity is independent of the input space dimension (Wolff, 2017; Awad and Khanna, 2015; Lawal and Kwon, 2021; Wang et al., 2013). The main idea of SVR is to use nonlinear transformation to map observations into a higher dimensional feature space and then solve the linear regression problem in that space (Zhang et al., 2018; Miranda et al., 2018; Bineshian et al., 2012).

Given an input sample $\mathbf{x} = [x_1, x_2, \dots, x_n]^T$ and its corresponding desired output y_i , the regression estimation function of the SVR can be expressed as follows:

$$f(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x}) + b \quad (7)$$

where $f(\mathbf{x})$ is the forecast value of the input sample, $\mathbf{w}$ is a vector of coefficients to be estimated, b denotes the bias, and $\phi(\mathbf{x})$ is the transformation function (Zhang et al., 2018; Miao et al., 2018; Peng et al., 2018; Alkroosh et al., 2015; Rostami and Kaveh, 2021). $\mathbf{w}$ and b are estimated by minimizing the following optimization problem:

$$\text{minimize } \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^n (\xi_i + \xi_i^*) \text{ subject to } \begin{cases} y_i - \mathbf{w}^T \phi(\mathbf{x}_i) - b \leq \varepsilon + \xi_i \\ -y_i + \mathbf{w}^T \phi(\mathbf{x}_i) + b \leq \varepsilon + \xi_i^* \\ \xi_i, \xi_i^* \geq 0 \end{cases} \quad (8)$$

where C denotes the penalty factor, ξ_i and ξ_i^* are slack variables, and ε is a

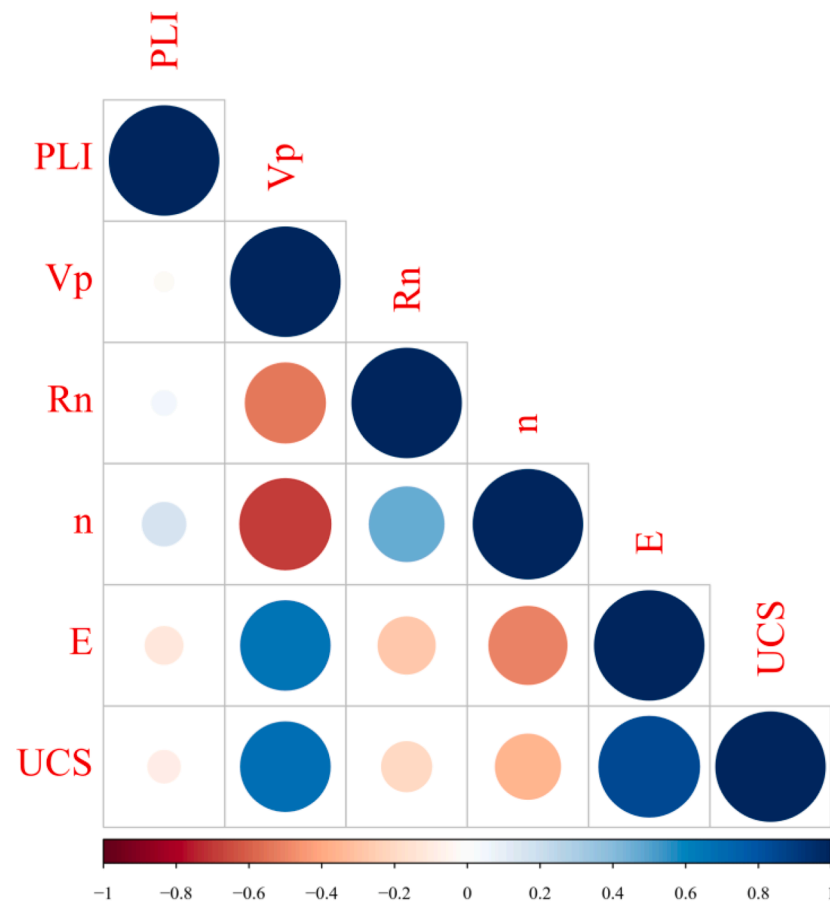


Fig. 3. Pearson correlation between rock properties and their representative mechanical indexes.

constant that specifies the radius of the tube (ε -tube) around the estimated function (Li et al., 2018; Panahi et al., 2020; Valera et al., 2018; He et al., 2019).

3. Results and discussions

3.1. Correlation assessments

SHAP values were used to rank variables based on their level importance for the UCS and E prediction and indicate their correlations. Results (Fig. 1) indicated that V_p and PLI had the highest and lowest effectiveness for predicting outputs, respectively. Assessing the magnitude of relationships showed that except n , which showed a negative correlation with the outputs, other variables illustrated a positive relationship with UCS and E (Figs. 1-2). There is a significant agreement between SHAP and Pearson correlation assessments (Fig. 3).

The strong relationship between V_p and mechanical properties of rock was reported in various investigations (D.J. Armaghani et al., 2016; Jamshidi et al., 2016; Lama and Vutukuri, 1978; Zezza, 1990; Valdeon et al., 1996; Goudie, 1999; Nicholson, 2001). Porosity, the ratio of void percentage to the total sample volume, could control the rock durability and effects on its UCS and E (Wendler, 1997; Korkanc, 2013; Alves et al., 2011; Yavuz, 2012). Porosity, pore types, and cementation (heterogeneity parameters) in rocks control V_p . It was reported that V_p decreases by increasing the porosity. Thus, increasing porosity should decrease the UCS and E, while by increasing the porosity, the physical weathering increases and make the rock less durable. The SHAP and Pearson relationship assessments confirmed this negative correlation (Fig 1 and 3). The positive inter-correlation between $I_s(50)$ and UCS and E has been

Table 3
The XGBoost parameter settings were used for the prediction of E and UCS.

Parameter	E	UCS	Range
Base learner	Gradient boosted tree	Gradient boosted tree	Gradient boosted tree- Linear booster
Tree construction algorithm	Exact greedy	Exact greedy	Exact greedy- Approximate greedy
Learning objective	Regression with squared loss	Regression with squared loss	Regression with: squared loss – squared log loss
Learning rate (η)	0.1103	0.1103	$\{0.001k k \in \{1, 2, \dots, 1000\}\}$
Lagrange multiplier (γ)	0	0	$\{k k \in \{0, 1, \dots, 10\}\}$
Number of gradients boosted trees	201	206	$\{k k \in \{1, 2, \dots, 500\}\}$
Maximum depth of trees	6	6	$\{k k \in \{0, 1, \dots, 30\}\}$
The minimum sum of instance weight (hessian) needed in a child	6	6	$\{k k \in \{0, 1, \dots, 10\}\}$
L2 regularization term on weights	0.98	0.98	$\{0.01k k \in \{1, 2, \dots, 100\}\}$
The initial prediction score of all instances (global bias)	10.37	10.37	$\{0.01k k \in \{1, 2, \dots, 2000\}\}$
Subsample ratio of columns for each level	0.6	0.6	$\{0.1k k \in \{1, 2, \dots, 10\}\}$
Maximum delta step we allow each leaf output to be	0 (There is no constraint)	0 (There is no constraint)	$\{k k \in \{0, 1, \dots, 10\}\}$

Table 4

Accuracy assessment for the testing phase of various models.

UCS RMSE	R ²	E RMSE	R ²	Method
1.719	0.981	0.216	0.986	Random Forest
8.953	0.481	0.999	0.697	Support Vector Regression
0.647	0.997	0.037	0.999	XGBoost

addressed in several investigations (Yasar and Erdogan, 2004; Yaşar and Erdoğan, 2004; Deere and Miller, 1966; Goudie, 2006; Hoseinie et al., 2012).

3.2. Prediction

XGBoost model was used for the generation of UCS and E predictive models. 80% of records from the entire dataset were randomly used for the training stage, and the rest of the samples were considered for the testing stage. The XGBoost hyperparameters were mostly based on the algorithm defaults, and the rest was defined by try and error using the Grid Search algorithm (Table 3). The XGBoost outcomes (Table 4)

showed that UCS and E could accurately predict based on the rock properties. For validation purposes, the same dataset samples were used to generate RF and SVR models for the UCS and E prediction. Results (Table 3) indicated that the XGBoost model could predict the UCS and E with higher accuracy than these two typical AI models (Fig. 4). By comparing various ML algorithms employed in this paper, it is worth noting that both RF and XGBoost are ensemble methods but not SVR. XGBoost is a boosting technique, while RF is a bagging method. XGBoost is more adaptable than RF and SVR. It enables the user to customize the objective function. It also needs less feature engineering. SVR performs well in high dimensional space due to the kernel trick, while RF has a high computational cost. Since XGBoost implements parallel processing, it has a low computational cost. In terms of bias and variance, RF and XGBoost have low bias and variance, while SVR has low bias and high variance. All three algorithms are capable of dealing with outliers and handling them (Fan et al., 2018; Huang et al., 2020; Lee et al., 2019). These outcomes released that SHAP-XGBoost, as a powerful XAI machine learning model, could successfully be applied for modeling, controlling, and maintaining problems within rock mechanics .

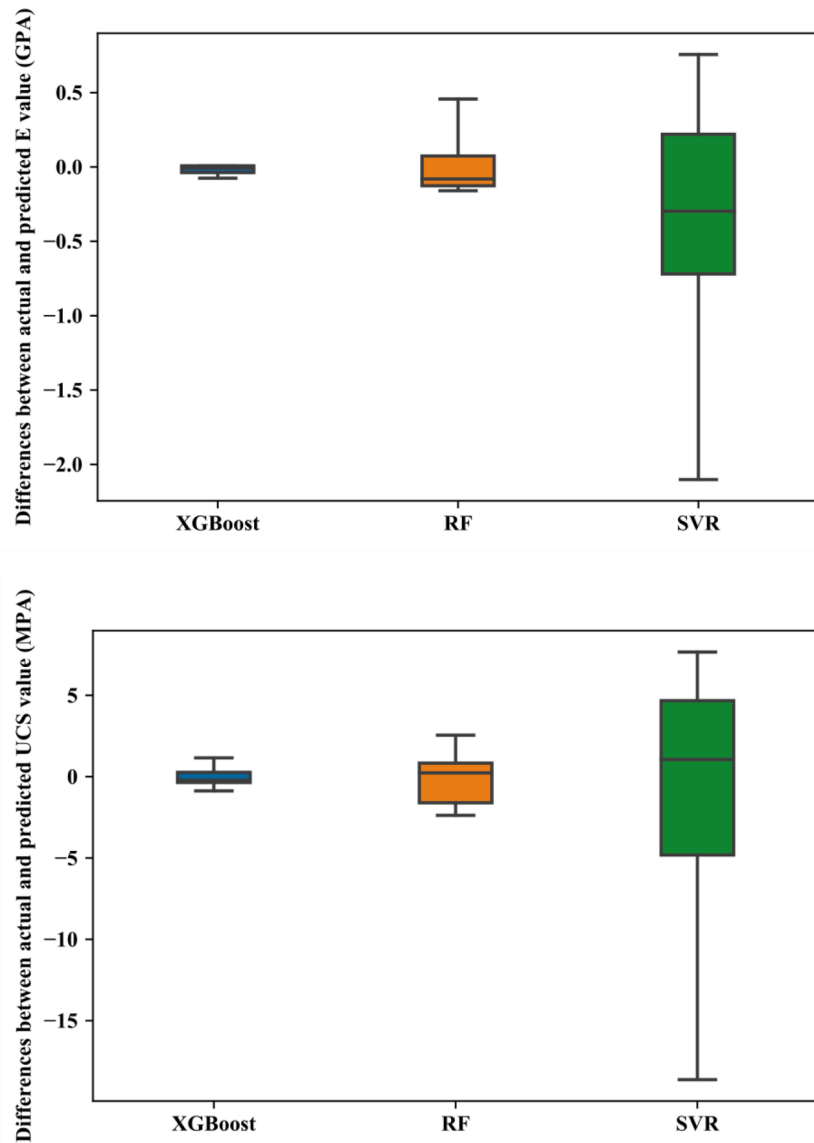


Fig. 4. Differences between actual and predicted UCS and E by different machine learning methods in the testing phase.

4. Conclusions

Outcomes of this investigation indicated that SHapley Additive ex-Planations (SHAP) as an explainable artificial intelligence method could accurately assess correlations between variables and illustrated the effect of each individual record of rock properties on the Travertine mechanical indexes (uniaxial compressive strength and modulus of elasticity). SHAP value indicated that P-wave velocity (V_p) has the highest impact on E and UCS modeling. While point load index, V_p , Schmidt hammer rebound number showed positive correlations with UCS and E, porosity illustrated a negative relationship based on the mean SHAP value. Modeling evaluation indicated that XGBoost could provide extensive UCS and E prediction results. The coefficient of determination of the predictive model for the UCS and E prediction was over 0.99. The estimation accuracy of XGBoost was higher than random forest and support vector regression based on statistical analyses. The SHAP-XGBoost results recommended that this modeling method be effectively used to understand and model challenging rock mechanics problems deeply.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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