Turkish Journal of Engineering

https://dergipark.org.tr/en/pub/tuje

e-ISSN 2587-1366

A comparative study to estimate the mode I fracture toughness of rocks using several soft computing techniques

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Keywords
Mode-I fracture toughness
Uniaxial compressive strength
Brazilian tensile strength
Soft computing techniques

Research Article
DOI: 10.31127/tuje.1120669

Received: 24.05.2022
Revised: 06.09.2022
Accepted: 23.10.2022
Published:27.02.2023

Abstract

Fracture toughness is an important phenomenon to reveal the actual strength of fractured rock materials. It is, therefore, crucial to use the fracture toughness models principally for simulating the performance of fractured rock medium. In this study, the mode-I fracture toughness (K_{IC}) was investigated using several soft computing techniques. For this purpose, an extensive literature survey was carried out to obtain a comprehensive database that includes simple and widely used mechanical rock parameters such as uniaxial compressive strength (UCS) and Brazilian tensile strength (BTS). Several soft computing techniques such as artificial neural network (ANN), adaptive neuro-fuzzy inference system (ANFIS), gene expression programming (GEP), and multivariate adaptive regression spline (MARS) were attempted to reveal the availability of these methods to estimate the K_{IC}. Among these techniques, it was determined that ANN presents the best prediction capability. The correlation of determination value (R^2) for the proposed ANN model is 0.90, showing its relative success. In this manner, the present study can be declared a case study, indicating the applicability of several soft computing techniques for the evaluation of K_{IC}. However, the number of samples for different rock types should be increased to improve the established predictive models in future studies.

1. Introduction

Fracture toughness is defined as a stress intensity factor (SIF) in fracture mechanics [1]. It also characterizes the resistance of materials against crack development. In terms of rock mechanics, it is a fundamental concept that provides a physical framework for understanding many processes associated with rock fractures. In a typical brittle material, three types of stress-strain states have been documented. Figure 1 shows a schematic plot of failure stress versus fracture toughness. For low toughness materials, brittle fracture is the governing failure mechanism, and critical stress varies linearly with fracture toughness, which is calculated using Equation 1 [2].

$$K_I = \sigma\sqrt{\pi a} \tag{1}$$

Where a is the radius of the crack plate, σ is the tensile stress causing the fracture in the material.

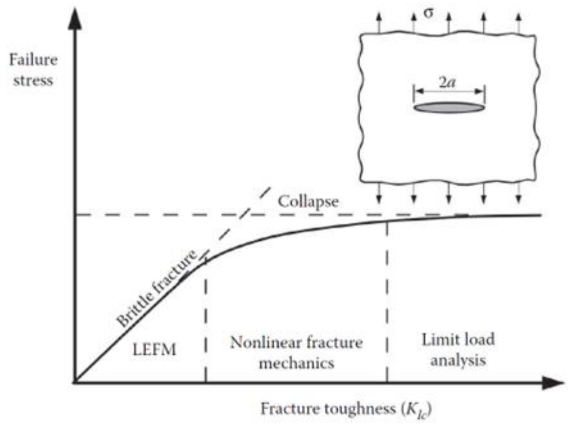

Figure 1. Effect of fracture toughness on the governing failure mechanism in a typical brittle material (LEFM: Linear elastic fracture mechanics, 2a: diameter of the crack plate, σ: tensile stress triggering fracture development) [2]

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Cite this article

Köken, E., & Koca, T. K. (2023). A comparative study to estimate the mode I fracture toughness of rocks using several soft computing techniques. Turkish Journal of Engineering, 7(4), 296-305

When the fracture toughness of the rock material increases, the principles of nonlinear fracture mechanics and limit load analysis are valid for the evaluation of various fracture types.

Based on modern rock mechanics and rock engineering approaches, three types of fracture toughness models have been identified, which are illustrated in Figure 2. Mode I fracture toughness (K_{IC}), where the principal load is applied normally to the crack plane, tends to open the crack. Mode II fracture toughness (K_{IIC}) corresponds to in-plane shear loading and tends to slide one crack face concerning the other. Mode III fracture toughness (K_{IIIC}) refers to out-of-plane shear. A cracked body can be loaded in any one of these modes, or a combination of two or three modes [2].

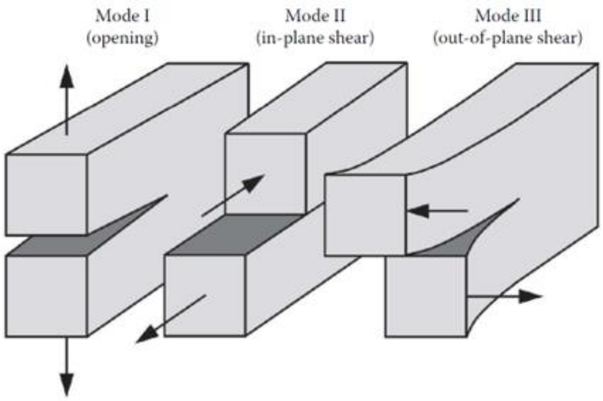

Figure 2. Three fracture toughness models in fracture mechanics [2]

Extensive scientific works have been carried out on the fracture toughness of rocks from different engineering geological aspects [3–12]. In these studies, the effects of elevated temperature, microwave treatment, and heating-cooling cycles on fracture toughness and the methods to determine the fracture toughness of rocks have been profoundly investigated. Regarding rock mechanics practices, the most common method to determine fracture toughness is based on using Brazilian disks with definite notches and cracked Chevron-notched Brazilian discs [13–21].

However, the determination of fracture toughness in the laboratory is laboring due to the requirement of special sample preparation and complicated testing procedures. Hence, several theories have been postulated to estimate the fracture toughness of rocks. Some empirical relationships to estimate the K_{IC} of rocks is listed in Table 1. However, the empirical relationships in Table 1 are valid for small-scale datasets or they represent a specific area of interest. Therefore, Pappalardo [22] described the regression-based predictive models as site-specific and he claimed that they have some limitations in dealing with larger datasets with different rock origins. To deal with larger datasets with different rock origins, soft computing tools would enable one to establish comprehensive predictive models. Based on a comprehensive literature survey, only two studies by Guha Roy et al. [23] and Afrasiabian and Eftekhari [24] proposed some soft computing-based predictive models for the evaluation of K_{IC} for different rock types (Table 2).

Table 1. Empirical relationships to estimate the K_{IC} of different rock types

Equation	R^2	Units	Ref.
$K_{IC} = 3.510^{-4} V_p^{-0.18}$	0.64	V_p in m/sec	[5]
$K_{IC} = 4.28\times10^{-3} UCS + 1.05$	0.30	UCS in MPa	
$K_{IC} = -0.50 n_e + 1.70$	0.36	n_e in %	
$K_{IC} = -0.332 + 0.000361 V_p$	0.96	V_p in m/sec	[25]
$K_{IC} = 0.0006147 V_s - 0.5517$	0.95	V_s in m/sec	
$K_{IC} = 0.02150 E_d + 0.2468$	0.93	E_d in GPa	
$K_{IC} = 3.2962 \gamma_d - 7.8974$	0.48	γ_d in kN/m^3	[26]
$K_{IC} = 0.0093 SHV^{1.2464}$	0.35	SHV and SH in numerical digits	
$K_{IC} = 0.0126 SH + 0.3644$	0.28		
$K_{IC} = -0.5304 \ln(BAV) + 2.5345$	0.61	BAV in cm^3/50cm^2	
$K_{IC} = 0.0408 \exp(0.0384 ISI)$	0.37	ISI in %	
$K_{IC} = 0.1331 PLI + 0.3921$	0.59	PLI in MPa	
$K_{IC} = 0.4075 \exp(0.1427 BTS)$	0.71	BTS in MPa	
$K_{IC} = 0.1013 UCS^{0.5038}$	0.36	UCS in MPa	
$K_{IC} = 0.0037 \exp(0.0022 \rho_d)$	0.54	ρ_d in kg/m^3	[27]
$K_{IC} = 0.45 V_p - 0.58$	0.55	V_p in km/sec	
$K_{IC} = 0.90 V_s - 1.06$	0.60	V_s in km/sec	

Explanations: V_p: P wave velocity, V_s: S wave velocity,
E_d: Dynamic Young modulus, UCS: Uniaxial compressive strength, n_e: Effective porosity, γ_d: Dry unit weight,
SHV: Schmidt hammer rebounding number, SH: Shore hardness, BAV: Böhme abrasion value, ISI: Impact strength index,
PLI: Point load index, BTS: Brazilian tensile strength,
ρ_d: Dry density

Table 2. Soft computing-based predictive models to estimate K_{IC} for different rock types

Data analysis method	R^2 Training	R^2 Testing	Independent variables	n	Ref.
ANN	0.87	0.91	BTS, V_p, V_s	45	[23]
FIS	N.R	0.92			
ANFIS	N.R	0.97			
GEP	0.88	0.57	UCS, BTS	60	[24]
	0.88	0.76	UCS, E		
	0.86	0.75	BTS, E		
	0.86	0.87	UCS, BTS, E		

Explanations: BTS: Brazilian tensile strength, V_p: P wave velocity, V_s: S wave velocity UCS: Uniaxial compressive strength, BTS: Brazilian tensile strength, E: Young Modulus, ANN: Artificial neural networks, FIS: Fuzzy inference system, ANFIS: Adaptive neuro-fuzzy inference system, GEP: Gene expression programming, N.R: Not reported.

It is clear to figure out that using soft computing tools for the evaluation of K_{IC} for different rock types has not been much studied. For this reason, the present study aims to build comprehensive predictive models for the evaluation of K_{IC} using several soft computing tools and also to find out their superiority over one another.

For this purpose, artificial neural network (ANN), adaptive neuro-fuzzy inference system (ANFIS), gene expression programming (GEP), and multivariate adaptive regression spline (MARS) were adopted as the data analysis methods. The datasets were compiled from various published literature, and they are transformed into a comprehensive database for soft computing analyses.

As a result, four robust predictive models have been developed as a function of the UCS and BTS of rock material. The robustness of the models was evaluated by the coefficient of determination (R^2) values.

The details and mathematical formulations behind the proposed models are also given in this study to let users implement them in their work more efficiently.

The present study, in this manner, can save time and provide accurate and practical information on the K_{IC} of different rock types and understand the physical interaction between the input parameters and the K_{IC}. The predictive models established in this study could also be integrated into rock mechanics applications such as hydraulic fracturing and drilling and blasting in fractured rock medium.

2. Data documentation

A comprehensive literature survey was conducted to compile quantitative data on the K_{IC} for different rock types. Unfortunately, a significant number of previous studies could not have been regarded due to a lack of information on physical and mechanical rock properties, which are so important as input parameters. As a result of the literature survey, a database composed of 60 cases including the UCS and BTS of rocks was developed (Table 3). Before involving the database in the soft computing analyses, the database was randomly divided into the training (70/100) and testing (30/100) parts. The soft computing analyses were first conducted using the training parts of the database then the models were verified using the testing part.

Table 3. Datasets employed in soft computing analyses

Rock type	UCS (MPa)	BTS (MPa)	K_{IC} (MPa $m^{0.5}$)	n	Reference
Limestone	105.0	2.3	0.40	1	[3]
Shale	12.0–16.0	0.86–1.07	0.15–0.22	2	[10]
Gabbro	132.5	11.1	1.97	1	[11]
Granite	151.0–157.4	9.7–12.0	1.60– 1.70	3	[18]
Limestone, Travertine, Marble, Trachyte, Basalt	43.3–145.9	3.3–9.6	0.60–1.80	15	[26]
Sandstone, Shale, Basalt, Tonalite	33.0– 145.2	5.4–19.4	0.30–3.50	6	[27]
Basalt, Syenite	148.6–222.	11.10–13.20	1.35–1.70	2	[28]
Sandstone, Limestone	32.3–144.9	2.7–8.5	0.30–0.90	3	[29]
Granite, Diorite, Marble, Sandstone, Limestone	40.0– 219.0	5.0–15.0	1.10–3.80	6	[30]
Granite	173.0–259.0	7.9–12.8	1.26–1.71	3	[31]
Diorite	211.0	14.9	3.8	1	[32]
Granite, Diorite	165.0–224.0	10.0–14.5	1.00–25.0	2	[33]
Diorite	165.0	14.8	3.30	1	[34]
Sandstone	32.0	3.6	0.28	1	[35]
Andesite, Marble	52.3–82.8	5.1–7.0	0.56–0.94	2	[36]
Marble	52.3–75.3	4.7–5.9	1.15–1.22	3	[37]
Pegmatite, Gneiss	105.0–123.0	10.0–14.0	1.9–3.1	3	[38]
Limestone, Rhyolite, Granite	55.0–240.0	10.7–12.2	0.80–1.21	3	[39]
Travertine	26.1–29.6	4.9–5.3	0.54–0.59	2	[40]

Explanations: UCS: Uniaxial compressive strength, BTS: Brazilian tensile strength, K_{IC}: Mode 1 Fracture toughness, n: Number of samples

Before performing the soft computing analyses, simple correlations of the considered variables were revealed by Pearson's correlation coefficient (r) and spearmen rho values, which are listed in Table 4. Accordingly, the UCS is moderately associated with the K_{IC}, whereas the BTS is highly correlated with the K_{IC}.

Therefore, these two independent variables can be readily selected as input parameters in soft computing analyses.

Table 4. Correlations of independent variables for the evaluation of K_{IC} for different rock types

Indicator	UCS	BTS
Pearson's correlation coefficient, r	0.595	0.829
Spearman rho value	0.689	0.811

3. Data analysis methods

3.1. Adaptive neuro-fuzzy inference system (ANFIS)

Considering many advantages, researchers have used ANFIS to build various predictive models that are many used in engineering geological problems [41–43]. The advantage of the ANFIS is that it practices a hybrid learning process to estimate the premise and consequent parameters [44].

In most ANFIS models, Sugeno fuzzy reasoning algorithm is primarily adopted based on numerous membership functions. Based on this information, the ANFIS analyses were carried out in the MATLAB environment in this study. The UCS and BTS of rocks were selected as input parameters for the evaluation of K_{IC} (Figure 3a). For each input parameter, three triangular membership functions were identified (Figure 3b, 3c). Then, nine different if-then rules were developed in the context of ANFIS analyses (Figure 3d). Finally, the ANFIS model structure was completed (Figure 3e) for interpretation. The if-then rules employed in the ANFIS analyses are listed in Table 5.

Table 5. If-then rules established in the ANFIS analyses

Rule	Description
1	If UCS is **in(1)** and BTS is **in(1)** then K_{IC} is **0.1889**
2	If UCS is **in(1)** and BTS is **in(2)** then K_{IC} is **0.7836**
3	If UCS is **in(1)** and BTS is **in(3)** then K_{IC} is **11.09**
4	If UCS is **in(2)** and BTS is **in(1)** then K_{IC} is **0.4918**
5	If UCS is **in(2)** and BTS is **in(2)** then K_{IC} is **1.747**
6	If UCS is **in(2)** and BTS is **in(3)** then K_{IC} is **3.206**
7	If UCS is **in(3)** and BTS is **in(1)** then K_{IC} is **8.582**
8	If UCS is **in(3)** and BTS is **in(2)** then K_{IC} is **0.2904**
9	If UCS is **in(3)** and BTS is **in(3)** then K_{IC} is **6.43**

3.2. Artificial neural networks (ANN)

ANN can analyze the data, learn and save the experience-based knowledge, and utilize it in future predictions [45, 46]. This parallel distributed learning algorithm is applicable to many problems, from social sciences to applied sciences. In most ANN models, a feed-forward backpropagation algorithm is adopted.

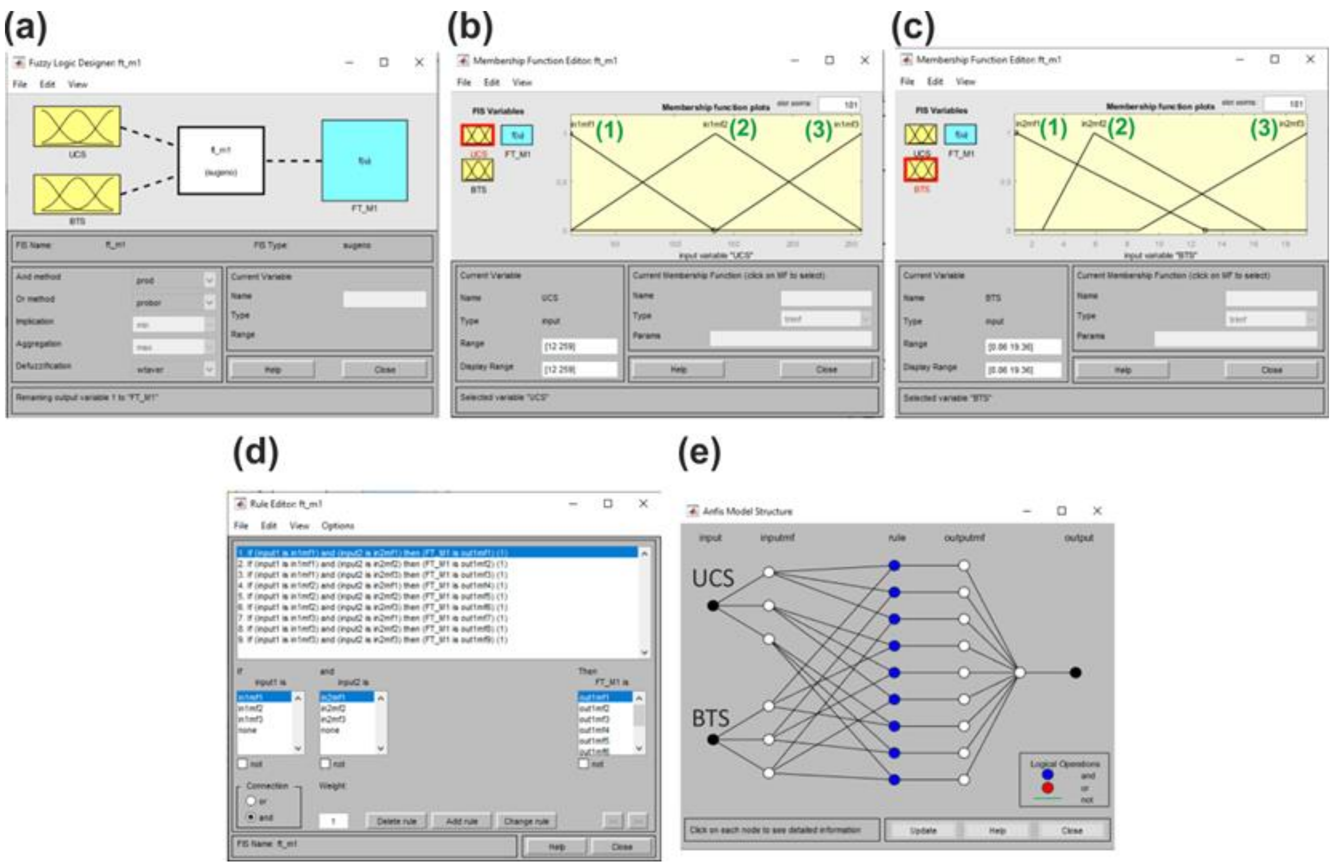

Figure 3. ANFIS outputs a) Input parameters b) UCS membership functions c) BTS membership functions d) If-then rule viewer e) ANFIS model structure

In this study, several ANN analyses were performed using the neural network toolbox (nntool) in the MATLAB environment. The novel ANN-based predictive model was introduced with definite mathematical equations using the weights and biases extracted from the ANN analyses. The ANN architecture adopted in this study is illustrated in Figure 4.

The UCS and BTs of rocks were adopted as input parameters. Six different hidden layers were developed in the ANN analyses and finally, a robust ANN model was developed to estimate the KIC of rocks.

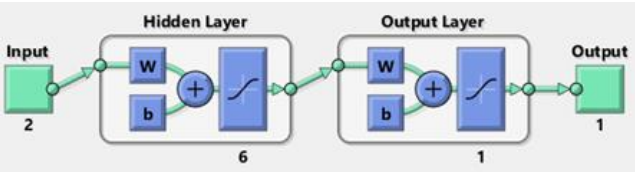

Figure 4. ANN architecture adopted in this study.

Before performing the ANN analyses, the database was normalized between −1 and 1 using Equation 2. As a result of the ANN analyses, K_{IC} can be estimated using Equation 3. The subfunctions of Equation 3 were determined based on the deterministic approach described by Das [47] and they are listed in Table 6.

$$V_n = 2\left(\frac{x_i - x_{\min}}{x_{\max} - x_{\min}}\right) - 1 \qquad (2)$$

where x_i is the relevant parameter to be normalized, x_{min}, and x_{max} are the minimum and maximum values in the dataset (Table 3).

$$K_{IC(ANN)} = 1.778\tanh\left(\sum_{i=1}^{6} x_i - 0.547\right) + 1.9177, R^2 = 0.90 \qquad (3)$$

Table 6. Subfunctions of the proposed ANN model

$x_1 = 2.9235\tanh\left(9.6091\,{}^{n}UCS - 4.0477\,{}^{n}BTS - 3.5939\right)$
$x_2 = -2.8967\tanh\left(12.2927\,{}^{n}UCS - 5.7981\,{}^{n}BTS - 4.9622\right)$
$x_3 = 0.39318\tanh\left(-4.2588\,{}^{n}UCS + 9.8239\,{}^{n}BTS + 3.9321\right)$
$x_4 = 0.91735\tanh\left(5.1937\,{}^{n}UCS - 2.3084\,{}^{n}BTS + 2.1721\right)$
$x_5 = -0.47452\tanh\left(-1.0616\,{}^{n}UCS - 13.8607\,{}^{n}BTS + 5.3417\right)$
$x_6 = 0.85583\tanh\left(-1.958\,{}^{n}UCS + 1.2956\,{}^{n}BTS - 0.55962\right)$
Normalization functions
${}^{n}UCS = 0.0081UCS - 1.0972$
${}^{n}BTS = 0.1081BTS - 1.093$

3.3. Gene Expression Programming (GEP)

The GEP is an evolutionary-based algorithm that produces an explicit mathematical formulation series between dependent and independent variables. The GEP was first developed by Ferreira [48], and for the past two decades, the GEP has gained popularity among researchers in various engineering fields.

In the context of the GEP models, the number of chromosomes, head sizes, and gene sizes were assigned to 10, 7, and 3, respectively. The linking function was the multiplication and root means squared error (RMSE) was regarded as the fitness function. As a result of GEP analyses, sub-expression trees are given in Figure 5. These sub-expression trees are also listed in Table 7 as mathematical formulations.

Table 7. Mathematical equations of the sub-expression trees

$x_1 = \frac{\left(-1.694 + \left(1 - BTS\right)\right)}{2} \times \min\left(\exp\left(-3.702\right); \frac{1}{UCS}\right)$
$x_2 = \min\left(BTS; \left(-0.552 - UCS\right)\right) + \min\left(UCS; BTS\right) + BTS$
$x_3 = \min\left(\frac{-1.851 + BTS}{2}; \frac{1}{BTS}\right) \times \exp\left(-4.378\right) \times 2BTS$

Based on the GEP model, the K_{IC} can be estimated using Equation 4 as follows:

$$K_{IC(GEP)} = 0.9415\prod_{i=1}^{3} x_i + 0.0721, R^2 = 0.73 \qquad (4)$$

3.4. Multivariate adaptive regression spline (MARS)

The MARS was firstly proposed by Friedman [49] as a nonparametric regression method, which can be perceived as a hybrid linear model. There are two important parts in typical MARS models. One is the forward pass and the other one is the backward pass. In the forward pass, MARS models are initiated with constant terms, which are called basis functions (BFs). On the other hand, in the backward pass, the BFs are connected with linear regression models. In this study, a novel MARS model was introduced to estimate the K_{IC} of rocks.

The MARS analyses were performed using the software R and the established MARS model is given as Equation 5. The BFs of the MARS model are listed in Table 8.

Table 8. BFs of the established MARS model

Basis functions	Equation
BF2	$\max\left(0; 11.18 - BTS\right)$
BF3	$\max\left(0; BTS - 9.57\right)$
BF5	$\max\left(0; BTS - 10.22\right)$
BF10	$\max\left(0; UCS - 144.9\right)$

$$K_{IC(MARS)} = 2.00 - 0.192BF2 - 1.336BF3 + 1.671BF5 + 0.0027BF10,\ R^2 = 0.75 \qquad (5)$$

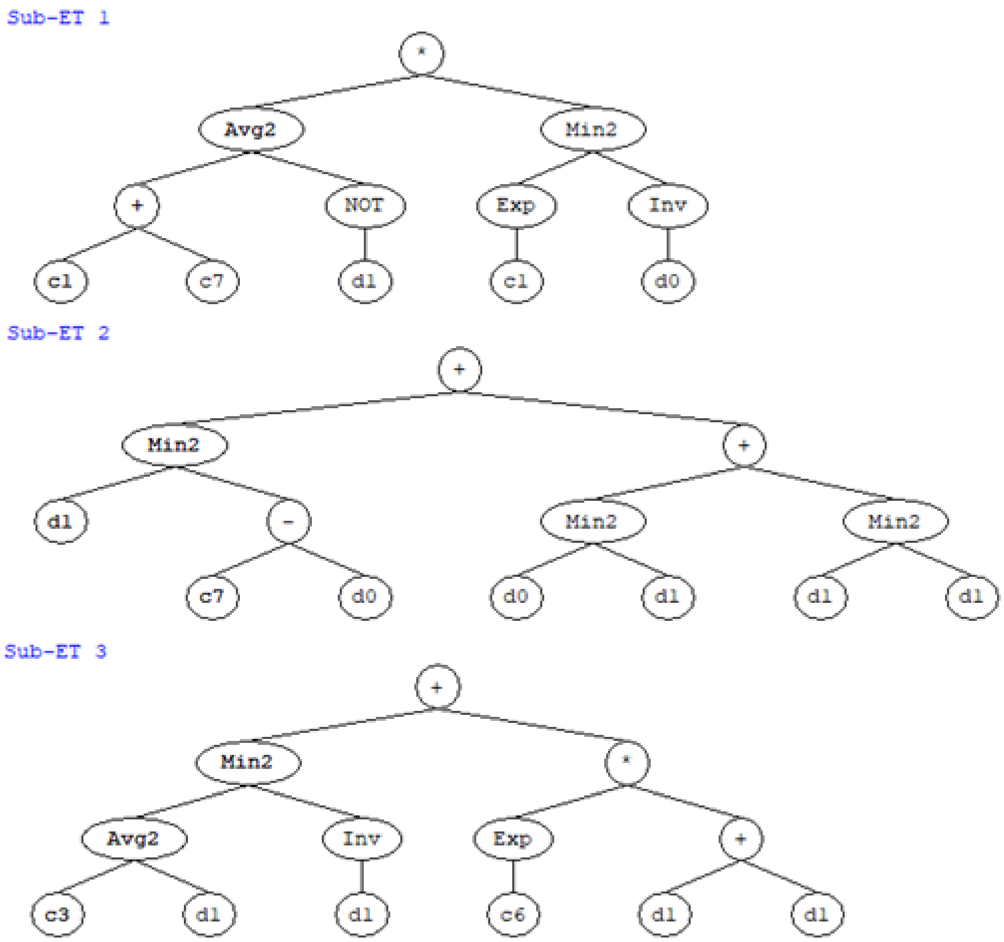

Figure 5. Sub-expression trees of the established GEP model (d0: UCS, d1: BTS, g1c1: –3.702, g1c7: 2.008, g2c7: –0.552, g3c3: –1.851, g3c6: –4.378)

4. Discussion

Simple regression models to estimate the K_{IC} of compiled rock types are illustrated in Figure 6. Accordingly, the BTS of rocks is highly associated with the K_{IC}. However, simple regression models are not enough for precise estimations. Therefore, soft computing analyses were performed to estimate K_{IC} values with intended accuracy. As a result of the soft computing analyses based on the database collected from rock mechanics test results (Table 3) presented in the literature by some researchers, four robust predictive models were developed to estimate the K_{IC} for different rock types. The predicted K_{IC} values by this study versus K_{IC} values compiled from the literature are plotted in Figure 7 for each model. Accordingly, the predicted and measured K_{IC} values are in good agreement which shows the model's relative success. The correlation of determination value (R^2) for the ANFIS, ANN, GEP, and MARS models was found to be 0.86, 0.90, 0.73, and 0.75, respectively (Figure 7).

The soft computing analysis results obtained from the present study indicated that the ANN model (Equation 3) is found to be the best predictive model for the evaluation of K_{IC}. This finding indicated the strong learning ability and adaptivity of the ANN methodology.

The soft computing models presented better R^2 values than most of the regression models proposed in the literature except for the regression models proposed by Zhixi et al. [25]. Because the regression models of these researchers were developed using 13 cases composed of several sandstone samples.

As it is well known, if the sample size decreases and it is distributed more evenly, the regression models may have a better prediction performance.

When comparing the performance of the established soft computing models with the ones previously proposed by Guha Roy et al. [23] and Afrasiabian and Eftekhari [24], it is clear to state that the proposed ANN model is better than the GEP models proposed by Afrasiabian and Eftekhari [24]. Nevertheless, the GEP model in this study was not as successful as the GEP model proposed by Afrasiabian and Eftekhari [24]. The reason for this phenomenon may be interpreted as the structure of the GEP model being quite different.

On the other hand, the proposed models presented a lower performance than the models proposed by Guha Roy et al. [23]. The reason for this phenomenon can be attributed to the fact that the dataset used in this study involves different rock types unlike the dataset of Guha Roy et al. [23] and also input parameters that were integrated into the soft computing analyses are different. It is certain that as the variety of the rock types increases, the model performances may decrease.

However, it can be claimed that the BTS of rocks can be a correlative parameter for the evaluation of K_{IC}. The Pearson's correlation analysis results also support this phenomenon (Table 4).

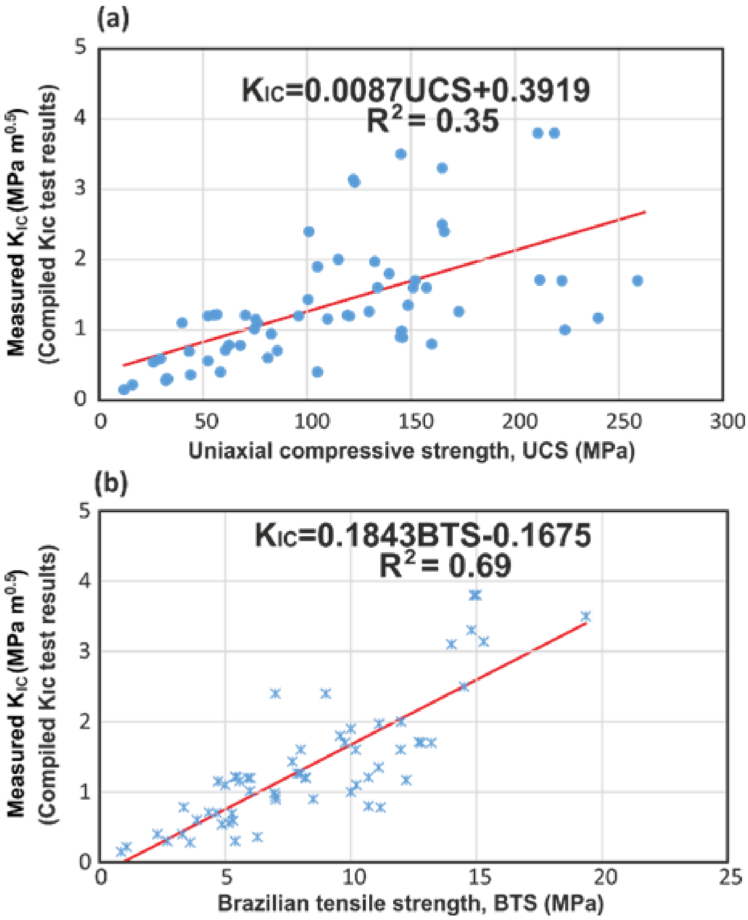

Figure 6. Simple regression models for the evaluation of K_{IC} based on different rock properties a) UCS b) BTS

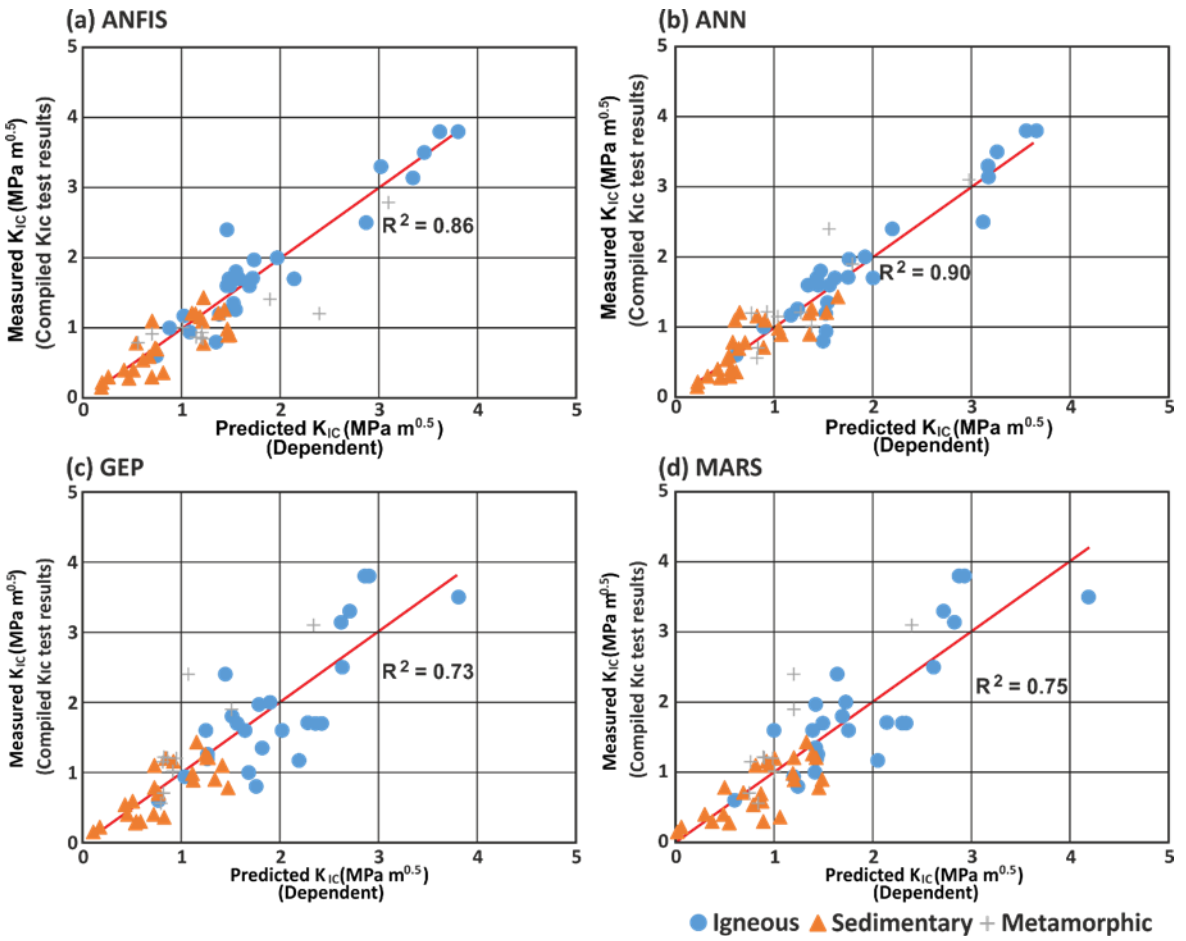

Figure 7. Predicted and measured K_{IC} values for the established models a) ANFIS b) ANN c) GEP d) MARS

On the other hand, the use of MARS models has not been previously used for estimating the K_{IC} for a wide range of rock types. It was found that although the MARS and GEP models provide lower performances than the ANFIS and ANN models, they might have the potential on estimating the K_{IC}.

Overall, the findings obtained from the present study and the ones from the previous studies indicated that the UCS, BTS, V_p, and V_s can be used to estimate the K_{IC} of rocks. In this study, only UCS and BTS of rocks were adopted since they are the most commonly measured parameters in engineering geological projects.

Since the ANN model was found to be the best predictive model among the models established in this study, an example of calculating the proposed ANN model was given as follows:

Example 1:
Case study 1 (Data was obtained from Reference 3)
UCS: 105.0 MPa, BTS: 2.3 MPa

Normalized values:

$$^{n}UCS = 0.0081 \otimes 105.0 - 1.0972 = -0.2467$$

$$^{n}BTS = 0.1081 \otimes 2.3 - 1.093 = -0.84437$$

Subfunctions:

$$x_1 = 2.9235 \tanh\ (9.6091 \otimes -0.2467 - 4.0477 \otimes -0.84437 - 3.5939) = -2.88438$$

$$x_2 = -2.8967 \tanh\ (12.2927 \otimes -0.2467 - 5.7981 \otimes -0.84437 - 4.9622) = 2.88494$$

$$x_3 = 0.39318 \tanh\ (-4.2588 \otimes -0.2467 + 9.8239 \otimes -0.84437 + 3.9321) = -0.39214$$

$$x_4 = 0.91735 \tanh\ (5.1937 \otimes -0.2467 - 2.3084 \otimes -0.84437 + 2.1721) = 0.91110$$

$$x_5 = -0.47452 \tanh\ (-1.0616 \otimes -0.2467 - 13.8607 \otimes -0.84437 + 5.3417) = -0.47452$$

$$x_6 = 0.85583 \tanh\ (-1.958 \otimes -0.2467 + 1.2956 \otimes -0.84437 - 0.55962) = -0.70559$$

$$K_{IC(ANN)} = 1.778 \tanh\ (-2.88438 + 2.88494 - 0.39214 + 0.91110 - 0.47452 - 0.70559 - 0.547) + 1.9177 = 0.43138 MPa\ m^{0.5} \text{ (Measured } K_{IC}\text{=0.40 MPa m}^{0.5}\text{)}$$

5. Conclusion

In this study, the K_{IC} of different rock types has been examined using ANN, ANFIS, GEP, and MARS methodologies. For this purpose, a comprehensive literature survey was conducted to compile such datasets for the implementation of the above-mentioned analysis methods. Consequently, 60 cases composed of the K_{IC}, UCS, and BTS of rocks from various published literature were considered. Based on the UCS and BTS of rocks, four robust predictive models have been developed.

Even though the ANN, ANFIS, and GEP models have been studied before for the evaluation of K_{IC}, the MARS model has not been used to estimate the K_{IC} of rocks.

Among these techniques, the ANN model (Equation 3) presented the best prediction performance. Contrary to the published literature, the GEP model has the lowest prediction capability with an R^2 of 0.73 for the evaluation of K_{IC}. The details and mathematical framework of the proposed models were introduced in this study to let users implement them more efficiently. The present study, in this context, can be declared a case study, indicating the applicability of several soft computing techniques for the evaluation of K_{IC}. However, the number of samples for different rock types should be increased to improve the established predictive models in future studies. Last but not least, it is important to note that the adopted techniques to estimate the K_{IC} of rocks may have some uncertainties due to their operational flow and the expert knowledge of the physical relationship between the input and output parameters.

Author contributions

Ekin Köken: Conceptualization, Methodology, Software, Writing-Original draft preparation **Tümay Kadakci Koca:** Writing-Original draft preparation, Validation, Editing.

Conflicts of interest

The authors declare no conflicts of interest.

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