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Prediction of Strength Parameters of Thermally Treated Egyptian Granodiorite Using Multivariate Statistics and Machine Learning Techniques

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Abstract: The mechanical properties of rocks, such as uniaxial compressive strength and elastic modulus of intact rock, must be determined before any engineering project by employing lab or in situ tests. However, there are some circumstances where it is impossible to prepare the necessary specimens after exposure to high temperatures. Therefore, the propensity to estimate the destructive parameters of thermally heated rocks based on non-destructive factors is a helpful research field. Egyptian granodiorite samples were heated to temperatures of up to 800 °C before being treated to two different cooling methods: via the oven (slow-cooling) and using water (rapid cooling). The cooling condition, temperature, mass, porosity, absorption, dry density (D), and P-waves were used as input parameters in the predictive models for the UCS and E of thermally treated Egyptian granodiorite. Multi-linear regression (MLR), random forest (RF), k-nearest neighbor (KNN), and artificial neural networks (ANNs) were used to create predictive models. The performance of each prediction model was also evaluated using the (R^2), (RMSE), (MAPE), and (VAF). The findings revealed that cooling methods and mass as input parameters to predict UCS and E have a minor impact on prediction models. In contrast, the other parameters had a good relationship with UCS and E. Due to severe damage to granodiorite samples, many input and output parameters were impossible to measure after 600 °C. The prediction models were thus developed up to this threshold temperature. Furthermore, the comparative analysis of predictive models demonstrated that the ANN pattern for predicting the UCS and E is the most accurate model, with R^2 of 0.99, MAPE of 0.25%, VAF of 97.22%, and RMSE of 2.04.

Keywords: Egyptian granodiorite; thermal treatments; predictive models; multivariate statistics; machine learning techniques

MSC: 62H10

1. Introduction

With the advancement of thermal engineering applications, such as geothermal energy extraction, deep nuclear waste storage, and coal mining, a more in-depth understanding of rocks' strength and index properties are essential. High-temperature conditions distinguish

these applications and may extend to 1000 °C, as in the coal gasification process [1]. Temperature can cause damage to the rock's surface and internal structure, which could induce instability and rock failure [2,3]. Moreover, during the evaluation process of the strength properties of rock, it is not always possible to extract drilled cores significantly to apply the destructive tests if the rock is deteriorated due to high-temperature exposure. Hence, it is crucial to develop alternative strategies to conduct a trial for recognizing the behavior of rocks after exposure to high-temperature circumstances. On the other hand, the rock's uniaxial compressive strength (UCS) and elastic modulus (E) are the two most critical rock properties in mining engineering applications. Hence, the strength parameters of rock material are essential for geotechnical engineering designs such as mechanical excavation, the design and construction of foundations, slope stability examinations, etc. [4–8]. Furthermore, UCS is one of the fundamental parameters used in the designing and planning stages [9] through rock mass classification systems, e.g., rock mass rating (RMR) [10,11], geological strength index (GSI) [12], and rock mass index (RMI) [13]. The direct estimation of UCS during the preliminary design step is too expensive, time-consuming, and complicated, mainly when conducting this test following standard procedures such as ISRM and ASTM [14–18]. The indirect evaluation of UCS supports mining engineers in overcoming the challenge of using traditional laboratory tests to calculate UCS and E. Therefore, the quick and inexpensive prediction of UCS and E from simple indirect tests that need limited preparation of the specimen through alternative and indirect methods, such as simple and multiple regression models and soft computing techniques, is an attractive trend for scholars [19–23], etc.

Many efforts have been made to forecast the UCS and E of different types of rock through various indices to individually reveal the correlation between the index and the predicted parameter by traditional regression [14,24–30]. However, there are many complexities in the application and generalization of the former statistical models, and it can be recommended only for specific rock types [5,31–33]. Furthermore, for several rock types, there is no agreement regarding the equations obtained from regression analysis. In addition, one disadvantage related to the update of statistical model equations concerning new data is that, when different from the original data, "site-specific data may be inappropriate for users to evaluate UCS and E in another site" [34–37]. Many recent studies have highlighted using soft computation techniques due to their feasible, fast, and promising means for resolving complex geotechnical engineering problems to surmount the challenges of these traditional techniques [38–40]. For instance, artificial neural networks (ANNs), Adaptive Network-based Fuzzy Inference System (ANFIS), Genetic Programming (GP), and Regression Tree methods in predicting UCS and E of rock in an objective and practical approach [15,21,22,35,41–60]. These methods are receiving more attention in resolving challenging rock engineering issues. As a result, numerous researchers use statistical approaches to extrapolate rocks' strength and informational qualities from their physical properties. In comparison to multilinear regression and the adoptive neural-fuzzy inference system, it has been suggested that an artificial neural network-based prediction model is the most effective model for measuring granite thermal damage factors based on porosity [61]. A prediction model for uniaxial compressive strength and the static Young's modulus utilizing multilinear regression, artificial neural networks, random forest, and k-nearest neighbor is proposed by [62] after evaluating the heat effect on the physical, chemical, and mechanical properties of marble rock. According to the results, MLR and ANNs provided R^2 values of 0.81 and 0.90 for MLR and 0.85 and 0.95 for ANNs for both ES and UCS, while E and UCS prediction have an R^2 of 0.94 and 0.97 for KNN and RF, respectively. As input variables for these characteristics, density, porosity, and ultrasonic wave velocities were used [63–65]. Such studies opine that the predictive abilities of artificial intelligence techniques outperform statistical methods. According to the results of these studies, soft computing techniques are more effective at predicting mechanical properties than statistical methodologies.

Rocks can be exposed to high temperatures and either slow or rapid cooling, such as after fires. Accordingly, the physical and mechanical properties of these rocks will be affected. In addition, Young's modulus and uniaxial compressive strength are crucial variables for the efficient design of engineering applications in rock mass environments. These two factors require labor-intensive and expensive laboratory analysis, and if the testing procedure is not carried out correctly, the results could be inaccurate. Furthermore, drilled cores may not always be significantly recoverable if the rock has been damaged by exposure to high temperatures. The tendency to estimate the destructive parameters of thermally heated rocks based on non-destructive parameters is a hot research topic and is very limited. Moreover, after performing an intensive literature review regarding the prediction of uniaxial compressive strength and Young's modulus of rocks under different thermal conditions based on non-destructive parameters (as illustrated in Table 1), it was seen that there are rare studies related to this research area. Thus, this paper uses different prediction models to predict the UCS and E based on the physical parameters of Egyptian granodiorite after thermal and cooling treatments. Predictive models were created using multi-linear regression (MLR), random forest (RF), k-nearest neighbor (KNN), and artificial neural networks (ANNs). The coefficient of determination (R^2), root mean square error (RMSE), mean absolute percentage error (MAPE), and variance accounted for (VAF) were used to assess the effectiveness of each prediction model. The findings of this research will make it simpler to efficiently deal with the rocks in engineering construction projects under high-temperature rock mechanics conditions and help to predict UCS and E without the need to estimate them in the laboratory.

Table 1. Summary of some recent related studies in various locations.

Rock Type (Region)	Reference	Conditions	Input Parameters	Output Parameters
Travertine (Haji a bad, Iran).	Dehghan et al., 2010 [49]	25 °C	V_p, n, I_s, SH	UCS, E
Carbonate rocks (southwestern Turkey).	Yagiz et al., 2012 [20]	25 °C	n, SH, I_d, V_p	UCS, E
Granite (Peninsular Malaysia).	Jahed et al., 2015 [22]	25 °C	ρ_{dry}, Qtz, Plg, V_p	UCS, E
"Gabbro, limestone, granite, sandstone, quartzite, tuff, diabase, etc. (Turkey)	Teymen, et al., 2020 [51]	25 °C	BTS, SH, SSH, I_s, V_p, UW	UCS
Basalt stones (Jordan)	Barham, et al., 2020 [60]	25 °C	ρ_{dry}, SH, BTS, I_d, I_s	UCS
limestone, sandstone, marl, and dolomite (Khewra Gorge)	Umer et al., 2020 [66]	200 °C	BTS, UCS	E_d
Granite (Pakistan)	Naseer et al., 2022 [61]	25–900 °C	ρ_{dry}, n, V_p	DT
Marble (Pakistan)	Naseer et al., 2022 [62]	25–500 °C	T, V_p, ρ_{dry}, n, E_d	UCS, E

P-wave velocity (V_p), porosity (n), point load index (I_s), Schmidt hammer (SH), slake durability index (I_d), dry density (ρ_{dry}), quartz content (Qtz), plagioclase content (Plg), Shore hardness (SSH), Brazilian tensile strength (BTS), unit weight (UW), and dynamic elastic modulus (E_d).

2. Rock Description and Experimental Data

2.1. Geological Setting

Granodiorite is an igneous rock that has recently been used in various projects such as ladders, hydro-engineering constructions, road paving materials, construction, and monuments. A silica-rich intrusion of magma that cools in batholiths beneath the surface produces granodiorite, a plutonic igneous rock. Tonalite and granodiorite are two granitoid rocks that make up Egypt's Arabian-Nubian Shield. They make up more than 40% of the subsurface system in the Sinai and Eastern Desert [67]. In terms of structure, granodiorite is an intrusive igneous rock similar to granite. However, it contains more plagioclase-feldspar than orthoclase-feldspar in appearance and varies in type from granitic to alkali granite and old granite, which is dark gray [68]. In Egypt's Eastern Desert, granodiorite samples were

collected from old granite (near Gabel Abu Marwa). The study region is located between $23°00'$ and $23°10'$ north latitudes and $33°17'$ and $33°28'$ east longitudes (130 Km southeast of Aswan, Egypt), as illustrated in Figure 1a.
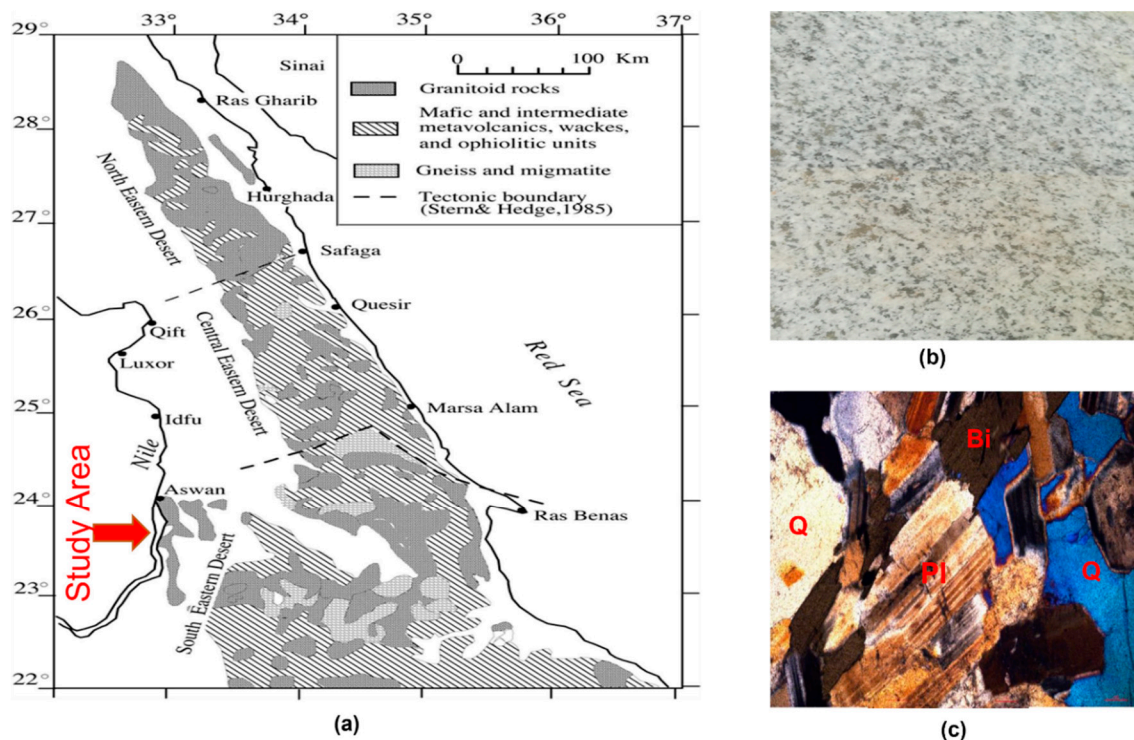

Figure 1. (**a**) Geological map of the studied area, (**b**) granodiorite appearance, and (**c**) a thin section micrograph of granodiorite.

2.2. Rock Description

The studied granodiorite samples were grey, as shown in Figure 1b, and had an average porosity of 0.54%, absorption wt. of 0.34, a dry density of 2610 kg/m^3, P-wave velocities of 5120 m/s, uniaxial compressive strength of 64 MPa, and Young's modulus of 48.8 GPa at room temperature. Employing a Bruker D8 Advance X-ray Diffractometer, X-ray diffraction (XRD) analysis revealed the rock's content to be quartz (Q), plagioclase feldspar (Pl), potassium feldspar (Kf), biotite (Bi), etc. (Figure 1c). Before testing, the samples were dried for at least 24 h at 105 °C.

2.3. Experimental Data

Based on the results obtained by Gomah et al. [2,69], the input and output data were used to build up the prediction models in this study. In these investigations, a high-temperature furnace (Nabertherm electric furnace-B410) with a thermal precision of ± 3 °C and a maximum temperature of 1300 °C was used for the heating process. Further, granodiorite samples were separated into five groups to ensure measurement accuracy, each with two subgroups of three samples for each target temperature. These groups were all then subjected to the same heating process. Granodiorite specimens were heated to the target temperatures of 200, 400, 600, and 800 °C, at a rate of 5 °C/min to prevent any potential thermal shock caused by the furnace's sharp thermal gradient. The temperature was held constant for 2 h, and the heated samples were then cooled to room temperature using slow cooling by natural air in the oven (hereinafter called slow-cooling samples or S-C samples) and rapid cooling by water (hereinafter called rapid-cooling samples or R-C samples), as illustrated in Table 2.

Table 2. Input and output data of prediction models.

Method	Temperature (°C)	Mass (g)	Density (g/cm^3)	P-Wave Velocity (m/s)	Porosity %	Absorption wt. %	UCS (MPa)	E (GPa)
				Input Data			**Output Data**	
-	25 °C	779	2.69	5619.82	1.33	0.50	66.9	50.7
		803	2.70	5645.16	0.00	0.00	65.9	47.8
		800	2.69	5633.80	1.35	0.53	59.2	48.0
S-C	200 °C	789	2.67	4455.88	1.20	0.46	66.3	41.1
		779.15	2.67	4450.37	1.29	0.50	67.1	44.1
		784.25	2.67	4454.55	1.25	0.48	67.6	43.0
R-C	200 °C	796	2.67	4039.74	0.00	0.00	70.2	41.8
		799	2.67	4070.00	1.27	0.51	71.6	50.2
		799.3	2.68	4050.00	1.29	0.50	67.4	45.1
S-C	400 °C	791	2.65	3482.81	1.32	0.51	75.9	31.5
		790	2.64	3495.68	1.43	0.56	67.9	28.9
		790.9	2.64	3384.83	1.32	0.51	73.9	31.2
R-C	400 °C	788	2.63	2911.69	0.00	0.00	55.0	24.7
		787	2.63	2606.52	2.48	0.98	56.1	25.1
		786.7	2.60	2613.88	2.57	1.00	69.3	26.5
S-C	600 °C	793	2.54	855.17	5.49	2.09	31.6	9.1
		793	2.54	1098.21	3.77	1.45	26.1	9.5
		783.9	2.54	815.49	5.17	2.03	26.8	8.6
R-C	600 °C	784	2.56	909.63	3.82	1.48	20.8	4.3
		783	2.42	754.55	3.80	1.45	19.4	3.9
		801.8	2.57	725.43	5.13	1.97	20.0	3.2
S-C	800 °C	787	2.24	0.00	10.85	4.17	2.7	-
		787	2.29	0.00	14.38	5.56	2.8	-
R-C	800 °C	786	2.22	0.00	16.88	5.64	1.5	-
		775	2.19	0.00	16.47	6.50	1.1	-

According to the International Society for Rock Mechanics (ISRM)'s suggested methods, the physical parameters of the granodiorite samples were calculated, both before and after the thermal treatments. Pundit PL-2 with two transducers (a transmitter and a receiver) was used as the ultrasonic pulse generator and acquisition system to quantify P-wave velocity along the specimen's axis [70]. R-C and S-C granodiorite samples underwent uniaxial compressive strength tests following the ASTM D7012-14 specifications. The mechanical properties were tested using a compression testing machine with a 200 T loading capacity. Two strain gauges were used, with a data-collection system linked to the device, to identify the axial and lateral displacements of the specimen. Finally, the mass, size, longitudinal wave velocity, absorption, porosity, UCS, and E of the granodiorite specimens were recorded and compared to their initial values after being subjected to different heating and cooling methods.

2.4. Prediction Models

2.4.1. Multiple-Linear Regression (MLR)

MLR is frequently employed to forecast relevant parameters. Simple linear regression, utilized in the case of numerous predictive variables, is expanded by MLR. Hence, it can be used to find the most pertinent and suitable equation when more than one independent variable is available as input parameters. In this study, a set of MLR was run using many independent variables to predict UCS and E. Equation (1) illustrates how it can describe the input without variables while considering how they relate.

$$Y = c + B_1X_1 + B_2X_2 + \ldots + B_nX_n \tag{1}$$

where the partial regression coefficients are B_1 to B_n, Y is the dependent variable, c is constant, and X_1 to X_n are the independent variables.

2.4.2. Random Forest Regression (RFR)

One of the most accurate prediction techniques for classification and regression among the numerous machine-learning algorithms is the emerging random forest (RF) algorithm, which was first implemented by Leo Breiman and Cutler Adele in 2001 [71]. This is because it can simulate complex interactions between input variables and thus is comparatively robust to outliers. The RFR algorithm has many benefits, including the ability to handle massive databases efficiently, the lack of sensitivity to noise or over-fitting [72], the ability to deal with thousands of input variables without deleting any, and the fact that it has lower complexity than other machine-learning algorithms (e.g., ANN). The RFR method is frequently used in geotechnical engineering [73]. For example, RFR was applied to the stability of rock pillars, and also in assessing landslide susceptibility and evaluating the potential for soil liquefaction [73–76].

The decision tree (DT) method and the bagging technique are the two fundamental parts of RF. The DT algorithm can be used for classification and regression issues depending on the dataset. The feature space is divided into smaller sections before applying the DT algorithm. Until the stop threshold is satisfied, the partitioning is carried out iteratively. Three parts—internal, external, and branches—are built when a DT is constructed. The internal nodes are constantly connected with decision-making functions to choose which node to contact next. The output nodes, also known as terminals or leaf nodes, are DT nodes that can no longer be split. The DT method is helpful in many civil engineering situations. However, the RF algorithm is more potent and reliable in many data mining tasks than a single tree [75]. RF is a technique for ensemble learning that builds on bagging to anticipate outputs [77]. Using various data from the bagging approach, several connected DTs are built in RF. The modeling accuracy is improving through the outcome averaging of all DTs, and overfitting is controlled. The overall structure of RF is shown in Figure 2, where n indicates the total number of trees built in RF and k1, k2, and kn are the outcomes of each DT.
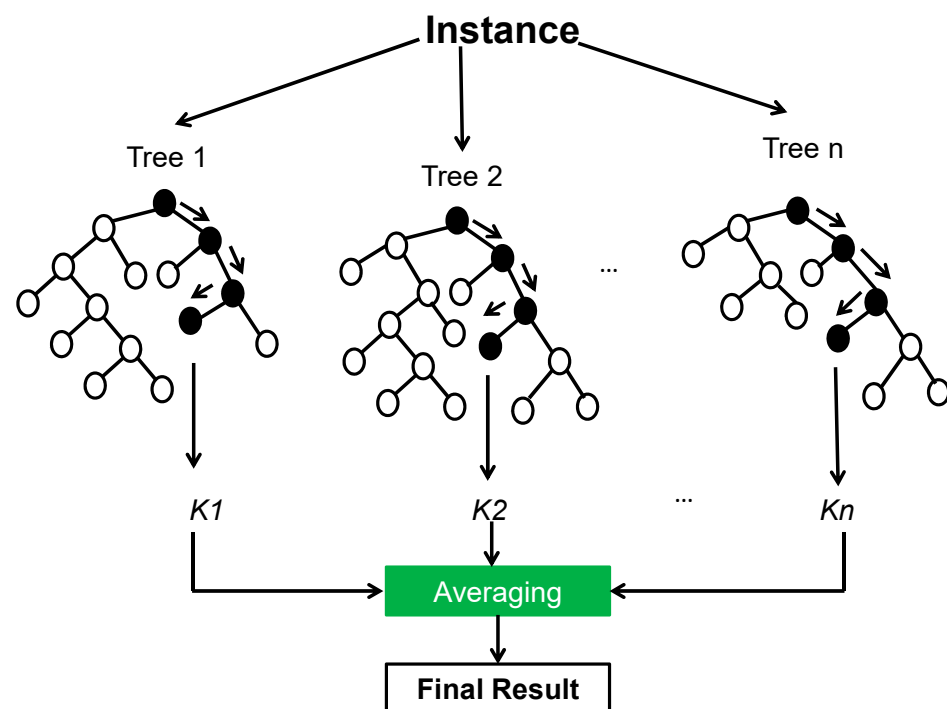

Figure 2. Fundamental design of the RF algorithm.

2.4.3. The K-Nearest Neighbor (KNN)

The labels of the K-nearest patterns in the data space are the foundation of nearest neighbor algorithms. In the context of large datasets and low dimensions, most relative

neighbor techniques are known to be effective local procedures. An extensive range of machine learning issues can be applied thanks to variations for multi-label classification, regression, and semi-supervised learning cases. The k-nearest neighbor (KNN) approach is easy to use, practical, and implementable [78]. This technique is utilized for classification and regression, much like ANN and RF. The fundamental idea behind KNN is to identify a set of "k" samples near unknown samples in the calibration dataset (for instance, by using distance functions). Finding collections of models that are identical to one another can help with this.

Furthermore, KNN establishes the category of unknown samples by averaging the relevant variables and contrasting the outcomes with the "k" samples. Because of this, the efficiency of the KNN depends significantly on the k value [79]. Employing the KNN approach has certain advantages, such as it being simple to understand and put into practice. Additionally, it can comprehend non-linear decision boundaries when used for classification and regression, and by varying the value of K, it can provide a very flexible choice limit. Additionally, there is not a phase in the KNN architecture solely for training; hence, adjusting the other hyperparameters is relatively easy. The three-distance function, which calculates the distance between nearby locations and is shown in the following Formulas (2)–(4), is used for the regression problem.

$$F(e) = \sqrt{\sum_{i=0}^{f}(x_i - y_i)^2} \tag{2}$$

$$F(ma) = \sum_{i=0}^{f}|x_i - y_i| \tag{3}$$

$$F(ma) = \left(\sum_{i=0}^{f}(|x_i - y_i|)^q\right)^{\frac{1}{q}} \tag{4}$$

where x_i and y_i represent the ith dimension, q indicates the order between the points x and y, and $F(e)$ stands for the Euclidean function. $F(ma)$ and $F(mi)$ are for the Manhattan and Minkowski functions, respectively.

2.4.4. Artificial Neural Network (ANN)

The artificial neural network is a soft computing technique that has recently been widely accepted as a predicting method in rock engineering applications such as tunnels, slope stability, and underground openings. ANN proffers better aptitudes in dealing with the nonlinear relationship between parameters than the traditional regression approaches. ANN models possess capabilities in processing the information pertinent to high parallelism and their ability to learn. Furthermore, solving the complex or imprecise data and grouping and filtration of noisy data to build the underlying correlation between the datasets [80] provide the extraordinary prediction efficiency of ANN models. Any artificial neural network is formed from several quite simple and highly interconnected processors, also neurons, due to their similarity to the biological neurons in the human brain [81,82]. A traditional ANN is usually represented by three principal components: network architecture, transfer function, and learning code [83].

Multi-layered perception (MLP) is employed in this section. It is made up of the following three layers: (1) an input layer for providing data; (2) a hidden layer using an algorithm and a set of features, neurons, and the hidden layer chosen through trial-and-error techniques [84]; and (3) an output layer for providing the input data's output. The number of neurons in each layer varies according to the application. Each link between a layer neuron and the one below it is connected and has weight [85]. The ANN model also employs several other algorithms. However, due to its straightforward training function, backpropagation (BP) is the most effective and is frequently utilized in engineering

challenges. Previous research has shown that the BP approach considers and presupposes a random value. The NN process uses that random value to calculate the result after that. Hence, the weight value will be changed to reduce the error margin. This process will be performed as often as necessary until the minimal result is achieved [86]. Supervised learning techniques must be employed throughout the training stage to guarantee the precision and efficacy of each classification and operation in ANN. The BP algorithm's networking is trained using a set of instances to connect and link the nodes and identify the parametric function, also known as weight inadequacies methods. The mean square error (MSE) is repeatedly reduced to reduce the difference between the actual and the predicted output. Training also helps in determining each iteration's weight.

This study produced a self-generated ANN code with n numbers of networks while maintaining the same training and activating function for a single loop, as illustrated in Figure 3. This code has a loop function that can run for many networks. Even though the data type may change, this code's essential activation function was constant, and the code was once run over 100 networks. The number of neurons for each network in a loop rose for each successor; as a result, network (1) had one neuron, network (2) had two, and so on. Several ANN algorithms are available; however, the recommendation [74] of using BP with the Levenberg–Marquardt algorithm is the most practical. Compared to other algorithms, Levenberg–Marquardt (LM) is more effective, requires a shorter time, and produces superior results. As a result, LM was applied to both the hidden and the output layers of the current model.
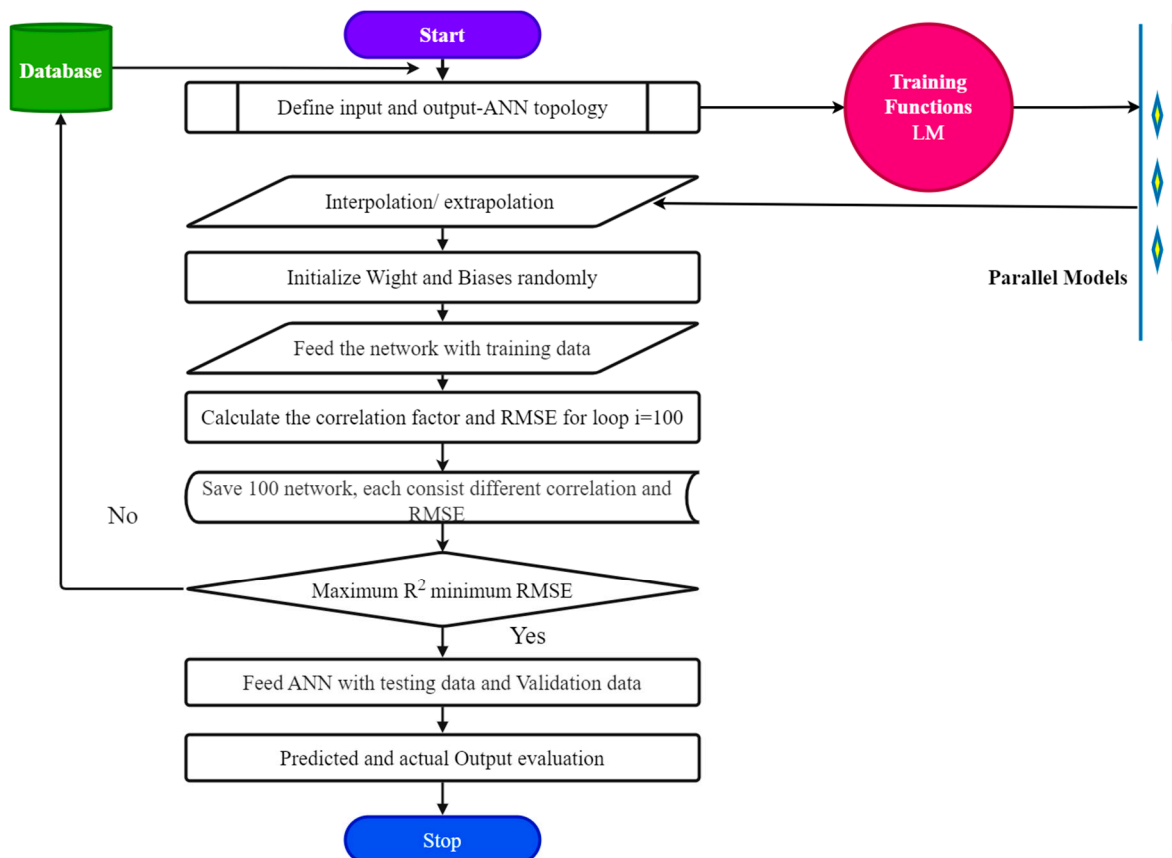

Figure 3. ANN flowchart for the UCS and E prediction model.

Figure 4 depicts an example of an ANN model's flowchart. A set of input layers, a predetermined number of hidden layers, and a bunch of output layers make up the usual ANN structure. The primary neuron is processed to estimate the output by linking the multiple layers of inputs with the proper weights (W) and biases (b). As shown, the basic structure of this analysis consists of two outputs (uniaxial compressive strength (UCS) and

elastic modulus (E)) and five inputs (temperature, absorption, porosity, dry density, and P-wave velocity). There was a total of 42 data points in the dataset. The following three categories of data were created: validation (15%), testing (15%), and training (70%).
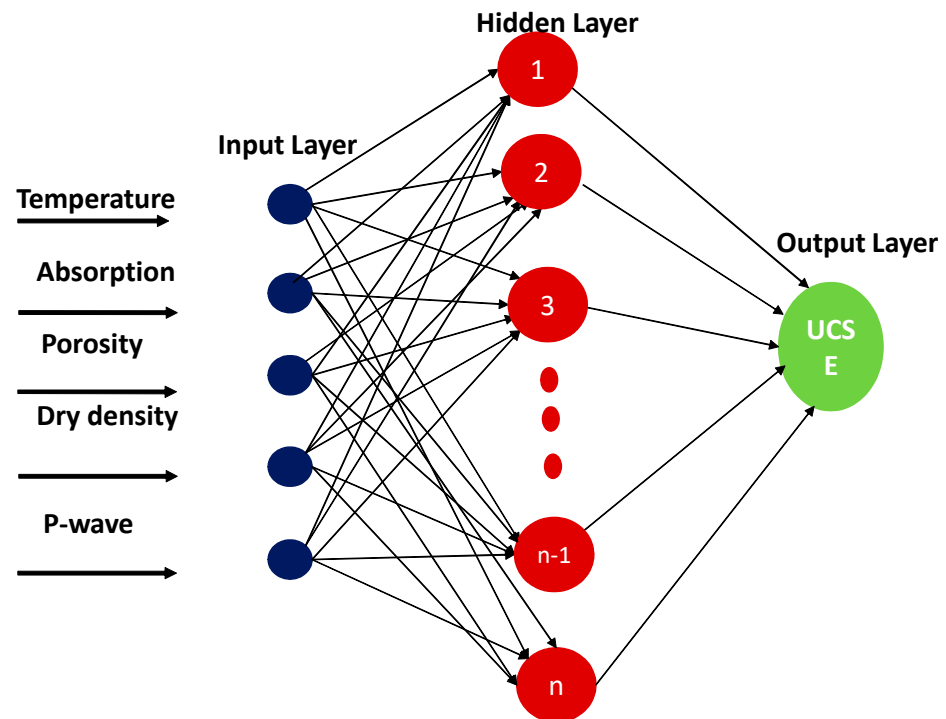

Figure 4. The structure of ANN for UCS and E predictions.

3. Results

3.1. Data Analysis

Thermal treatment significantly impacts the rock porosity and, consequently, water absorption of granodiorite. The porosity of the granodiorite specimens generally increased steadily for the both rapid- and slow-cooling methods, with temperatures rising but at different rates. Changes in linked mass and volume are the most significant influence on rock density. After being heated, the granodiorite's density gradually reduced compared to room temperature. Furthermore, thermal treatments significantly affected the granodiorite's ultrasonic wave velocities, and that behavior was noticed for both cooling methods studied. Summary of findings: The P-wave velocity of rocks decreases concurrently with temperature increases. Due to the severity of the thermal fissures, it was impossible to quantify the longitudinal wave velocity at 800 °C (assumed 0 m/s). Consequently, the degradation of the longitudinal wave velocity of granodiorite is caused by the physical and chemical alterations that occur after 600 °C, as displayed in Figure 5.

On the other hand, the mechanical properties of Egyptian granodiorite deteriorate primarily under the influence of temperature as the thermal expansion of its minerals change through their microstructure. Because of the mismatched growth during heating, thermal stresses are produced inside the granodiorite. When thermal stresses within or between minerals exceed the maximum strength of the minerals, microcracks and microfractures initiate and expand because thermal treatments induce mineral growth and chemical reactions [87]. As opposed to slow-cooled samples, rapid-cooled samples generally had lower uniaxial strength and elastic modulus, proving that the created microstructural alteration resulted from the thermal treatments and cooling methods, as shown in Figure 5. At 800 °C, the effects of high temperatures grew increasingly noticeable for both cooling techniques, and inter- and trans-granular cracks quickly developed, creating a network of microcracks. Furthermore, the granodiorite specimens' internal structures were destroyed, making them impossible to measure E (Table 1).
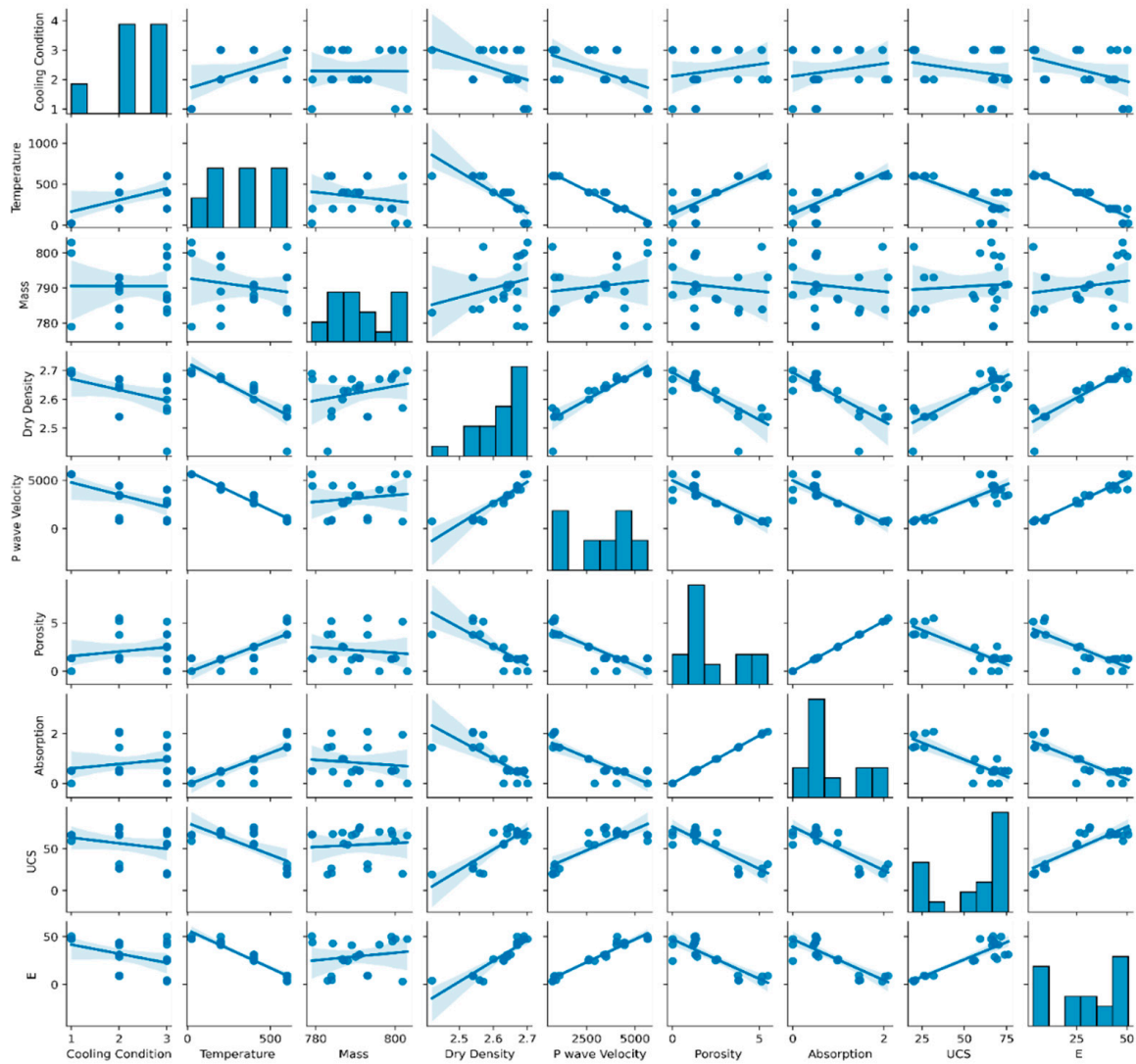
Figure 5. Input and output distributions as a pairwise correlation matrix.

For machine learning and statistical techniques, the parameters used in this work include the cooling method, temperature, mass, P-wave velocity, density, porosity, absorption, UCS, and E. The prediction of UCS and E is meant to employ the other parameters as inputs. Using a correlation matrix, a descriptive statistical technique, users may learn more about the variance and covariance of the regressions, which are part of the prediction model. Alongside other statistical matrices, it is frequently utilized. The correlation matrix typically explains each variable's fluctuation. Figures 5 and 6 can demonstrate this using correlation and paired correlation. The relationships between the input variables and the output include negative, positive, or no connections. For instance, variables that exhibit a negative correlation include temperature, absorption, and porosity. In contrast, the P-wave velocity and density had positive relations, while the mass and cooling method revealed poor relations with UCS and E. As they have a poor impact on both USC and E, as shown in Figure 6, the cooling method and mass of specimens were excluded from the following machine learning prediction as input parameters. Furthermore, after 600 °C, the model efficiency was minimized due to many input and output parameters being corrupted, such as Pv and E. Figures 5 and 6 make it simple for a researcher to grasp the impact of inputs on the expected model's output findings. The larger the negative or positive link, the more critical the model efficiency.
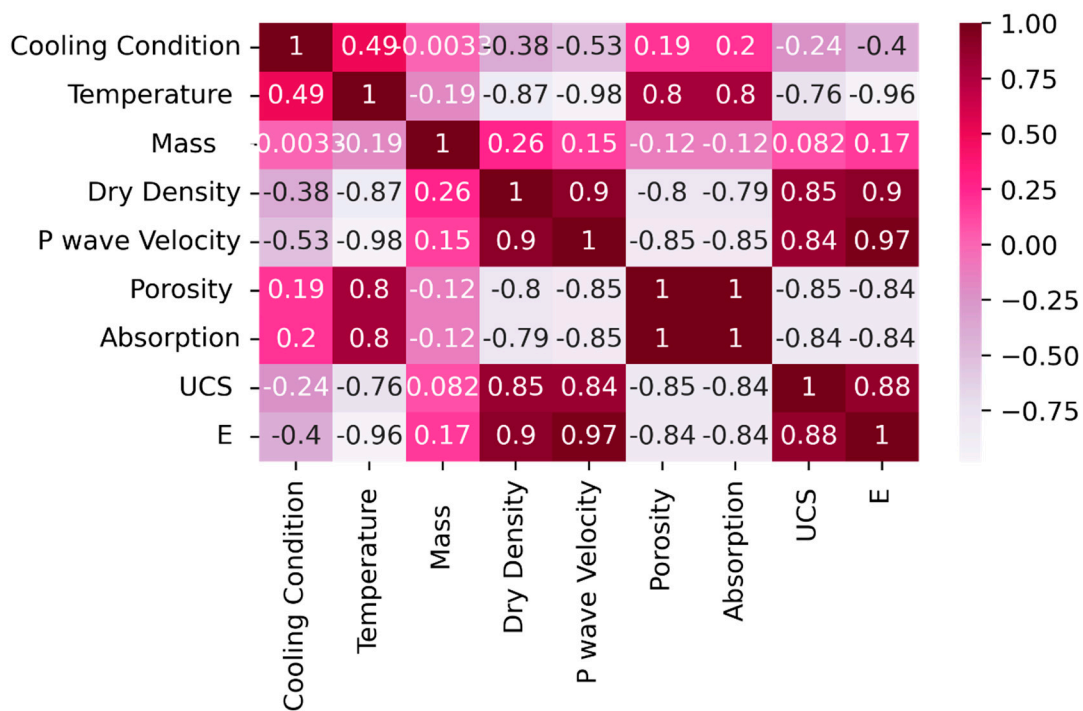
Figure 6. Inputs and outputs correlation matrix.

3.2. Model Performance

This study used statistical (MLR) and intelligent models (RFR, KNN, and ANNs) to create predictive models for the UCS and E of Egyptian granodiorite. The performance of predicted models is then investigated by comparing the correlation efficiencies of various generated models. The efficiency indices (R^2), (MAPE), (VAF), and (RMSE) were used to perform the evaluations for this comparison. The accuracy of model fitting is evaluated by the coefficient of determination (R^2). The linear fit equation represents this, and is defined as the ratio of actual data variation to estimated value variance. Less than 30% is regarded as suspicious, above 75% is regarded as remarkable, and a model with an R^2 of at least 55% is accepted. In addition, the efficiency of a prediction system is measured by the mean absolute percentage error (MAPE), also known as the mean absolute percentage deviation (MAPD). It can be expressed as the average absolute percent inaccuracy for every period, minus the actual values divided by the true values, and it describes this accuracy as a percentage. The standard deviation of the residuals is represented by the root mean square error (RMSE) (prediction errors). In a perfect scenario, the RMSE would be zero, a common indicator of the discrepancies between predicted or expected values and actual values. The variance accounted for (VAF) is typically used to verify that the predictive model is accurate. This is accomplished by comparing the outputs as anticipated and measured [88]. A VAF rating of 100 indicates that the predictive model accurately predicts the outcome. Consequently, the more accurately the forecast is made, the closer the predictive model's VAF is to 100 (i.e., lower variance). Hence, $R^2 = 1$, MAPE = RMSE = 0, and VAF = 100% are performance indicators that can be used to describe an outstanding model. Equations (5)–(8) were used to compute the performance indices, as shown below:

$$R^2 = \frac{\sum_{i=1}^{n} (y_i)^2 - \sum_{i=1}^{n} (y_i - k_i')^2}{\sum_{i=1}^{n} (y_i)^2} \tag{5}$$

$$\text{MAPE} = \frac{1}{2} \sum_{i=1}^{n} \left| \frac{y_i - k_i'}{y_i} \right| \times 100 \tag{6}$$

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}(y_i - k_i')}{n}} \tag{7}$$

$$\text{VAF} = \left[1 - \frac{var(y - k')}{var(y)}\right] \times 100 \tag{8}$$

where (y) is the actual value and (k') is the predicted value.

3.3. Prediction Models of UCS and E

3.3.1. Multilinear Regression Prediction Models

Two distinct multilinear regression equations were created for the prediction of UCS and E. Equations (9) and (10) can be used to express these mathematically, as follows:

$$\text{UCS} = -259.79 + 12.93\,Temp + 0.20\,density + 35.21\,velocity + 0.04\,porosity + 7.69\,Absorption \tag{9}$$

$$\text{E} = -62.51 + 5.02\,Temp - 0.003\,density + 16.12\,velocity + 0.01\,porosity + 4.50\,Absorption \tag{10}$$

A coefficient of determination (R^2) of 0.86 for the relationship between actual and predicted UCS (Figure 7a) and 0.96 for the relationship between actual and predicted E (Figure 7b) indicate the relation between actual and predicted UCS and E.
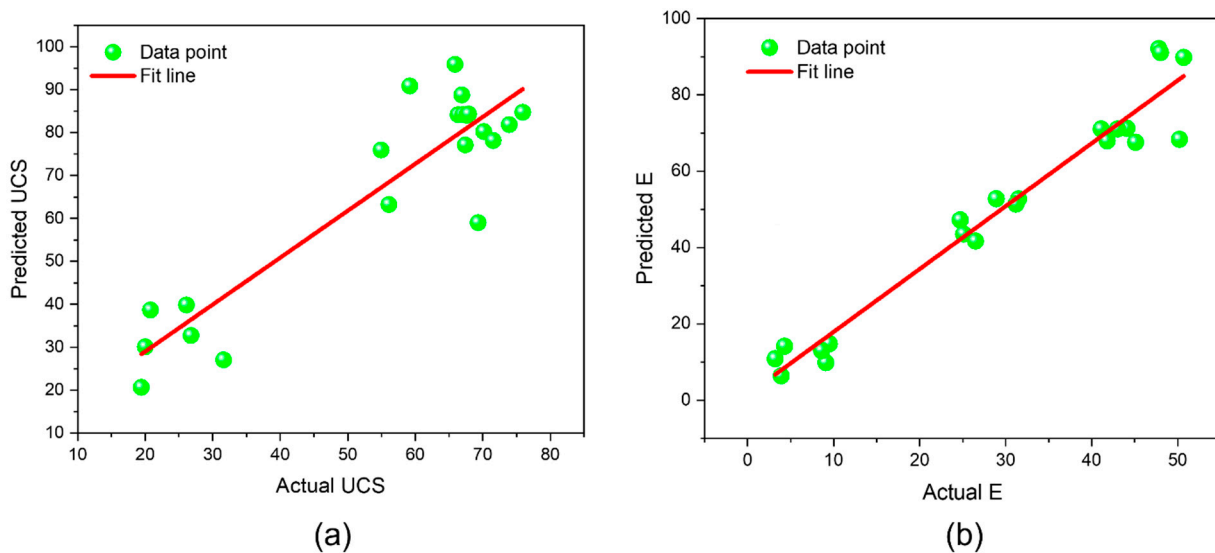

Figure 7. MLR model for actual and predicted UCS (**a**) and E (**b**).

3.3.2. Random Forest Technique

The random forest (RF) and k-nearest neighbor's regressions (KNN) models were built using Python's Scikit-Learn module. The python package includes many machine-learning techniques readily usable in various applications. The data were normalized to convert the values collected on diverse scales to a standard scale at the beginning of this analysis. Following that, 70% of the data were used to train the models, and the remaining 30% were divided into the testing set (15%) and the validation group (15%). With the aid of the testing set, the hyper-parameters were adjusted. The RF model's (n estimators) and (max depth) hyperparameters were varied throughout a range of possible values. The number of estimators, which is directly linked to the number of decision trees built by the random forest regression model, is determined before computing the maximum averages of forecasts. As the number of trees rises, the model becomes more computationally expensive while offering better performance. The max depth hyperparameters indicate the depth of every decision tree in a random forest. Because the max depth hyperparameter was allocated a very high value, the model is overfitted. Table 3 lists the ideal values

for n estimators, max depth, and random state. Additionally, as seen in Figure 8, the predicted values for USC and E have a strong correlation coefficient (R^2 = 0.98) for the actual parameter value.

Table 3. Optimized RFR hyperparameters.

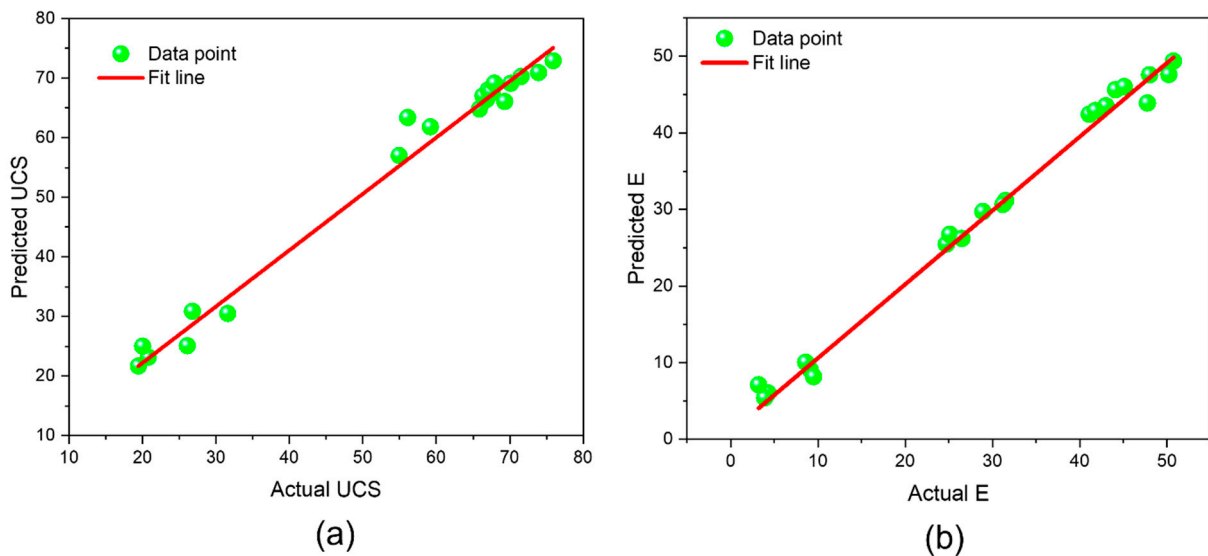| Parameters	Values	Details
n-estimators	100	Number of trees in RFR
Max-depth	12	Maximum depth of tree
Random state	10	Random state

(a)

(b)

Figure 8. Relationship between the predicted and actual UCS (**a**) and E (**b**) of Egyptian granodiorite using random forest technique.

3.3.3. K-Nearest Neighbor Technique

The variable "n neighbors" in the KNN model represented the number of neighbors, which might vary. The "number of neighbors" hyperparameter determines the number of neighbors that should be considered while averaging data for a forecast. The approach becomes more accurate and computationally costly when the value of the n neighbors hyperparameter is raised to a large amount. A grid search strategy was applied to find the ideal values for the hyperparameters. The grid search strategy tests a wide range of potential values for each hyperparameter being adjusted before choosing one to represent the perfect combination. The value was experimented with on various levels, while other hyperparameters stayed the same to establish a workable limit for each hyperparameter. The optimum pairing of n neighbors and metric values is described in Table 4. Additionally, as can be observed in Figure 9 that the predicted value at this parameter-optimal value has a good correlation coefficient (R^2 = 0.95) for both USC and E.

Table 4. Optimized KNN hyperparameters.

Parameters	Values	Descriptions
n-neighbors	11	Number neighbors
Metric	Minkowski	The distance metric to use

3.3.4. Neural Network Model

Figure 10 displays the regression values for the UCS and E models of granodiorite during each phase of the ANN, including training, validation, testing, and regression results.

Excellent regression was obtained during training, validation, and testing combinations between the predicted and measured measurements of UCS and E.
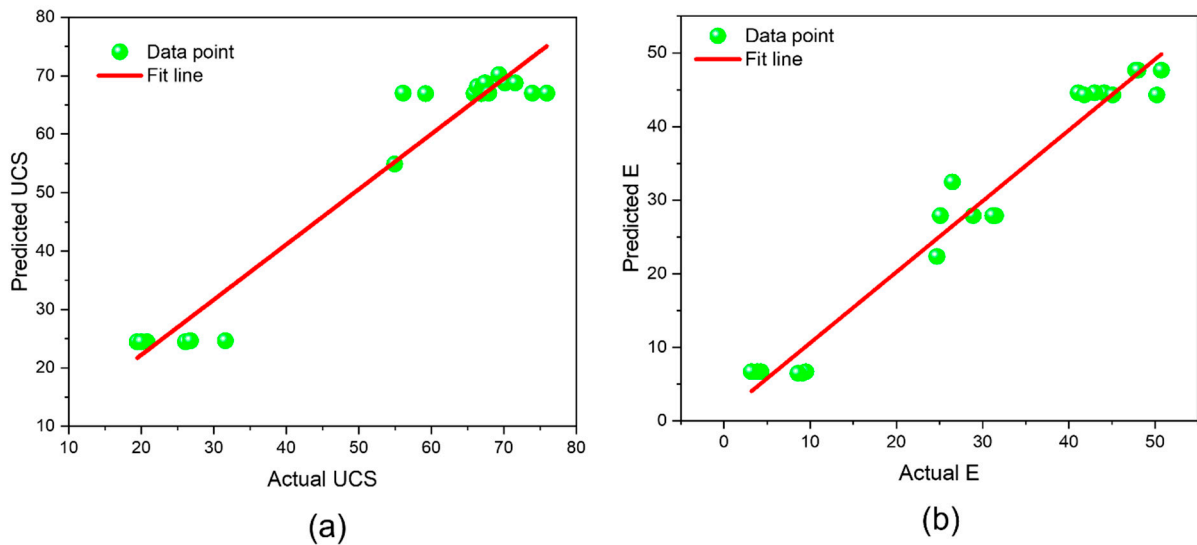

Figure 9. Relationship between expected and real UCS (**a**) and E (**b**) based on the KNN approach.
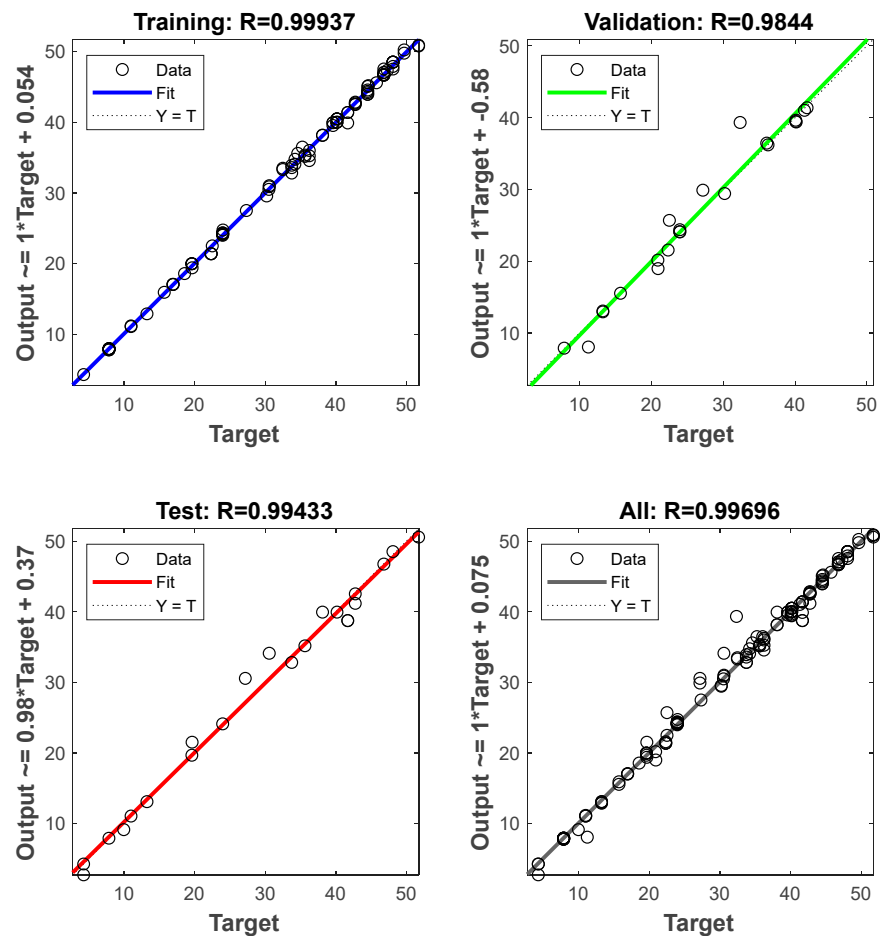

Figure 10. ANN training, validation, and testing stages with the related regression coefficient for UCS and E.

Consequently, as shown in Figure 11, an exceptional R^2 value (0.99) between the expected and actual (UCS and E) data is observed (Table 5).
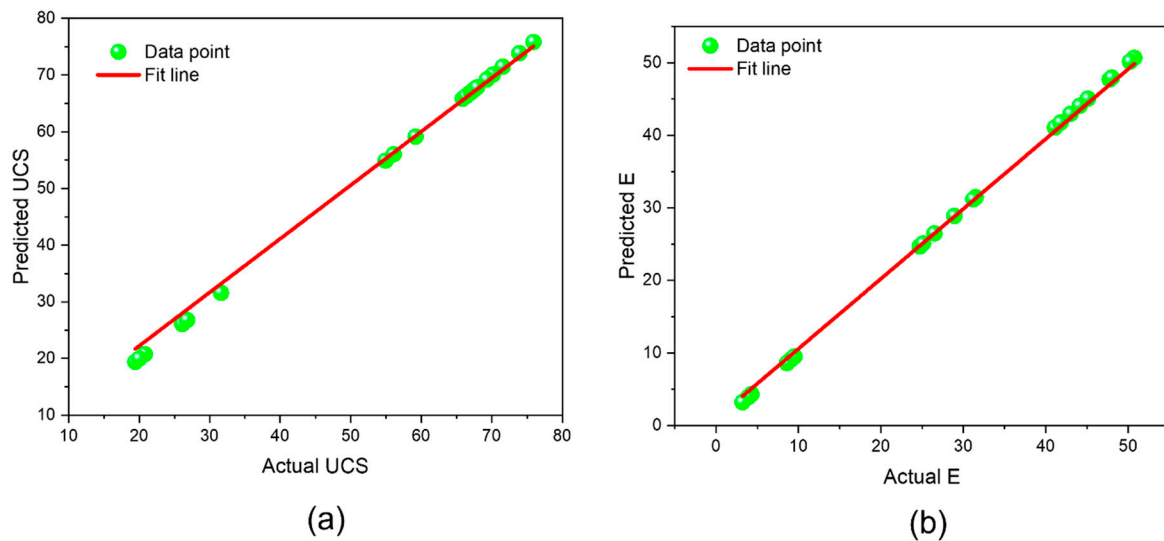

(a)   (b)

Figure 11. Relationship between the predicted and actual UCS (**a**) and E (**b**) using ANN approach.

Table 5. Relation between the actual and the predicted values of UCS and E for used intelligent methods.

Temperature (°C)	Actual UCS (MPa)	Actual E (GPa)	Predicted UCS (KNN)	Predicted E (KNN)	Predicted UCS (RFR)	Predicted E (RFR)	Predicted UCS (ANN)	Predicted E (ANN)
25 °C	66.85	50.73	66.95	47.68	66.43	49.38	66.79	50.68
	65.89	47.75	66.95	47.68	64.85	43.90	65.82	47.70
	59.2	48	66.95	47.68	61.84	47.59	59.14	47.95
200 °C	66.34	41.1	68.16	44.60	67.02	42.44	66.27	41.06
	67.08	44.1	68.16	44.60	68.04	45.64	67.01	44.06
	67.64	43	68.16	44.60	67.61	43.53	67.57	42.96
	70.15	41.8	68.78	44.30	69.13	42.91	70.08	41.76
	71.56	50.2	68.78	44.30	70.28	47.62	71.49	50.15
	67.41	45.1	68.78	44.30	67.75	46.05	67.34	45.05
400 °C	75.92	31.5	67.02	27.90	72.93	31.17	75.84	31.47
	67.91	28.9	67.02	27.90	69.17	29.72	67.84	28.87
	73.93	31.2	67.02	27.90	70.95	30.65	73.86	31.17
	54.95	24.7	54.89	22.35	57.02	25.47	54.89	24.67
	56.11	25.1	67.03	27.90	63.40	26.75	56.05	25.07
	69.32	26.5	70.20	32.48	66.10	26.21	69.25	26.47
600 °C	31.61	9.1	24.66	6.48	30.51	9.11	31.58	9.09
	26.11	9.5	24.49	6.70	25.10	8.16	26.08	9.49
	26.8	8.6	24.66	6.48	30.89	10.04	26.77	8.59
	20.79	4.3	24.49	6.70	23.17	6.02	20.77	4.30
	19.44	3.9	24.49	6.70	21.70	5.41	19.42	3.90
	20.01	3.2	24.49	6.70	25.01	7.11	19.99	3.20

The MSE (mean squared error) metric was used to assess network accuracy and efficiency. Increasing the neuron count in the hidden layer reduced the MSE value as the number of iterations rose. The MSE for each UCS and E model was assessed. A lower MSE number at 11 epochs for UCS and E resulted in the best regression model, as illustrated in Figure 12.
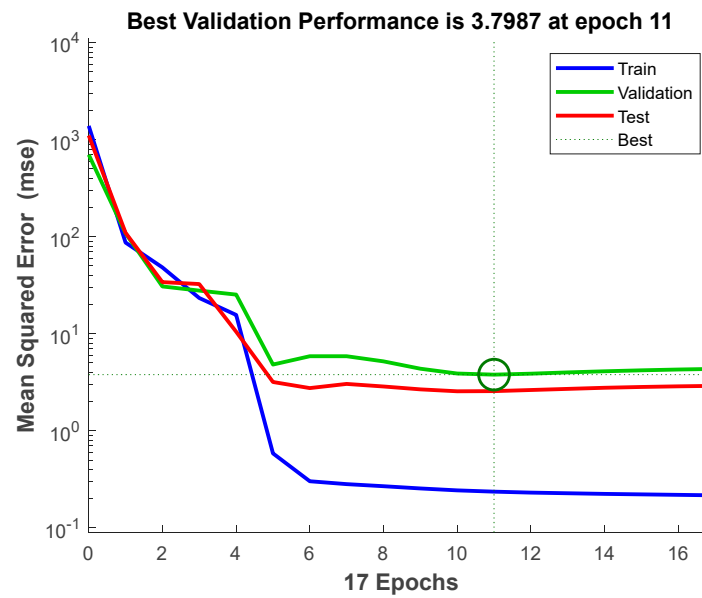
Figure 12. ANN Performance based on the mean squared error metric.

According to the neuron convergence investigation, as seen in Figure 13, the UCS and E best regression and least MSE were achieved on 17 neurons. This demonstrates that the number of iterations and the number of neurons critically influence the model's accuracy.
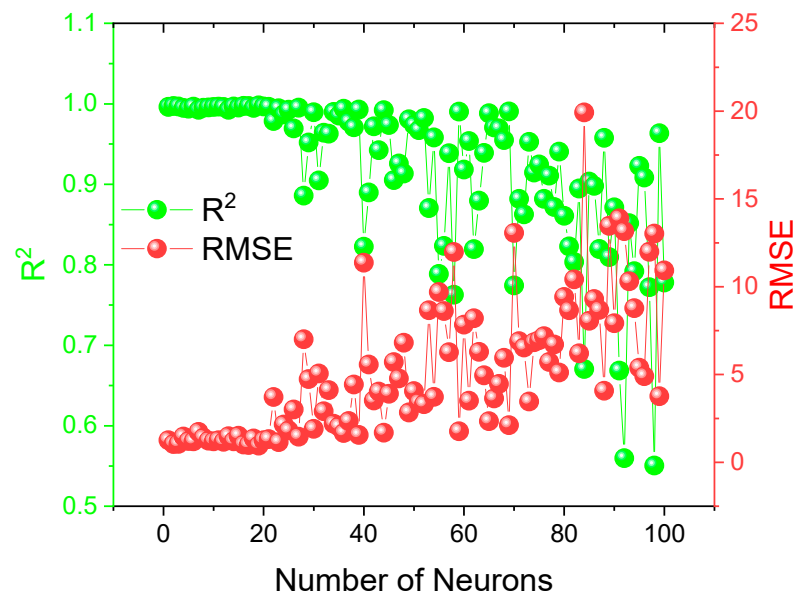

Figure 13. Impact of neuron convergence in the hidden layer.

4. Discussion

Thermal treatment causes mineral expansions and chemical reactions, which results in the formation and propagation of microcracks and microfractures. Mineral grains grow, and the thermal expansion characteristics of distinct minerals vary. Anisotropic thermal expansion along separate crystallographic axes of the same mineral under heating further contributes to uneven growth. Furthermore, the evaporation of free and constitutional water raises the micro-pores in granodiorite, which could affect the texture, such as in damage to the mineral silicate frame. As a result, microcracks occur between or inside the mineral grains. Hence, this can cause mineralogical, physical, and mechanical changes in rocks significantly different from those at room temperature.

Testing the UCS and E to gain more knowledge about the mechanical behavior of rock is more difficult in high-temperature deep geotechnical applications. Therefore, a more critical research aspect is the propensity to evaluate the destructive parameters of thermally treated rocks based on non-destructive factors. The UCS and E are thus predicted in this paper using various prediction models derived from the physical characteristics of Egyptian granodiorite following thermal and cooling treatments. The cooling technique, temperature, mass, P-wave velocity, density, porosity, and absorption to forecast the UCS and E were the input parameters used in this study. Prediction model effectiveness was reduced after 600 °C because many input and output variables, such as Pv and E, were hard to measure due to severe degradation to granodiorite specimens. As a result, the prediction models were built up to this critical temperature, which can be considered a threshold temperature point. The relationships between the input and the output variables indicated negative, positive, or no relations. In the prediction models, temperature, absorption, and porosity are factors that have a negative connotation. On the other hand, the density and P-wave velocity were positive. However, the mass and cooling technique demonstrated weak relationships with UCS and E; hence, they were eliminated from the soft computing prediction models. Moreover, as illustrated in Figure 6, temperature and P-wave velocity actively contributed to the elastic modulus prediction model. On the contrary, porosity, absorption, and density showed a less significant predictive impact. In contrast, porosity and density were the most efficient characteristics for predicting uniaxial compressive strength.

The greater the magnitude of the negative or positive relationship, the more crucial the model performance. As demonstrated in the results in Table 6, the MLR prediction models' performance coefficients for UCS and E are 0.86% and 0.96%, respectively. In contrast, intelligent models for UCS and E, such as RFR, KNN, and ANN, have higher performance coefficients of 0.98%, 0.95%, and 0.99%, demonstrating that their models for UCS and E prediction are more rational than the statistical model. Hence, the obtained results from this study are better than those concluded by [62]. Furthermore, after comparing the results obtained from the statistical (MLR) and soft computed models, it is concluded that the intelligent models perform better at predicting UCS and E than the MLR, whereas ANN provides a high coefficient of determination for UCS and ES, and the MLR provides a lower coefficient for both predicted parameters. Hence, based on these performance indexes, the ANN performed excellently.

Table 6. Performance indices of the developed models.

Predicted Parameter	Models	R^2	RMSE	MAPE (%)	VAF (%)
UCS	MLR	0.86	27.15	34.53	81.02
E		0.96	0.90	23.15	31.53
	RFR	0.98	0.14	1.18	94.23
UCS, E	KNN	0.95	3.02	0.94	94.01
	ANN	0.99	2.04	0.25	97.22

5. Conclusions

This article suggests a new predictive model quantifying the preheated Egyptian granodiorite's uniaxial compressive strength and its elastic modulus. Four prediction models were created: multi-linear regression (MLR), random forest (RF), k-nearest neighbor (KNN), and artificial neural networks (ANNs). These models were developed using five input parameters as a base (temperature, porosity, absorption, density, and p-wave). Each prediction model's efficiency was evaluated using the coefficient of determination (R^2), root mean square error (RMSE), mean absolute percentage error (MAPE), and variance accounted for (VAF). The principal conclusions are listed as follows:

(1)　Due to the close results of the slow cooling by the oven and rapid cooling by the water of thermally treated granodiorite, the cooling method and mass as input parameters to predict UCS and E have a minor effect on the prediction models of UCS and E. In

contrast, the temperature, porosity, absorption, dry density, and P-wave velocity had good relations with UCS and E.

(2) After 600 °C, the performance of the prediction models was diminished because many input and output parameters, such as Pv and E, were impossible to measure due to the severe damage to granodiorite samples. The prediction models were therefore developed up to this threshold temperature, which can be regarded as a threshold temperature point.

(3) The inconsistent performance for the MLR model demonstrates that the temperature and P-wave velocity actively contributed to the prediction models of elastic modulus. In contrast, the porosity, absorption, and density had a less significant predictive impact. In comparison, porosity and density were the best effective parameters to predict the uniaxial compressive strength.

(4) The performance coefficients for the MLR prediction models for UCS and E are 0.86% and 0.96%, respectively. In contrast, the intelligent models for UCS and E, including RFR, KNN, and ANN, provide a better performance coefficient (9–13%), indicating that their models for UCS and E prediction are more reasonable than the statistical model (MRL).

(5) The comparative analysis of predictive models revealed that the ANN model used for predicting the UCS and E is the most accurate model, with R^2 of 0.99, MAPE of 0.25%, VAF of 97.22%, and RMSE of 2.04.

Recommendation: This study mainly discusses three artificial intelligence techniques (RFR, KNN, and ANNs) and a conventional linear regression model (MLR). Other methods, such as the adoptive neural-fuzzy inference system (ANFIS model), may be employed to predict the mechanical parameters based on the non-destructive parameters. Moreover, as well known, rocks' chemical, physical, and mechanical behavior vary by region. This study examined Egyptian granodiorite. Hence, the study could be more general by considering different rocks in other locations. Moreover, future research may incorporate the sparse principal component analysis (PCA), one of the most commonly operated unsupervised machine learning algorithms for dimensionality reduction and visualize multidimensional data.

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