

Prediction of compressive strength of concrete at high heating conditions by using artificial neural network-based Bayesian regularization

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Abstract: Cement concrete is the most commonly used material today for constructing residential or commercial buildings, industrial parks, or particular components such as tunnel slabs where there is a high risk of fire. This structure requires concrete to be subjected to high temperatures generated by fires. However, concrete under the influence of high temperature has very complex behavior states with deformations, physical and chemical changes as the temperature rises dramatically. In this study, an artificial neural network-based Bayesian regularization (ANN) model is proposed to predict the compressive strength of concrete. The database in this study includes 208 experimental results synthesized from laboratory experiments with 9 input variables related to temperature change and design material composition. The performance of the ANN model was evaluated using K-fold cross-validation and statistical criteria, including mean absolute error (MAE), root mean square error (RMSE), and coefficient of determination (R^2). The results show that the proposed ANN model is a reasonable, highly accurate, and useful prediction tool for saving time and minimizing costly experiments.

Keywords: Machine learning, ANN, compressive strength, Bayesian regularization, K-fold cross-validation

1. Introduction

Due to its non-flammable properties and low thermal gradient, concrete is known to perform well at high temperatures, ensuring that thermal transients propagate slowly inside structural elements. Nonetheless, high-temperature microstructural transformations in concrete involve complicated physicochemical processes in the component. On concrete, high temperatures cause two primary concerns. One

is the damage of concrete's mechanical properties, which includes physicochemical variations in the binder and aggregate, thermal differences between the aggregate and the cement matrix as a temperature level and rate, applied force, and outer coating, which reduces evaporation from the concrete's surface. At higher temperatures, an exact number of physicochemical changes appear in the material: physically-compounded H_2O is delivered over

100°C; dioxolane hydrate dissociates over 300°C; calcium hydroxide hydrolyzed over 500°C; and several aggregates begin transferring or disintegrate at various temperatures (delivery of adsorbed H₂O, quartz SiO₂-conversion, limestone decomposing). Simultaneously, the second issue is concrete spalling. Ordinary concrete spalls due to fast temperature rises (about 20°C/min) [1]. In the transition zone between these two stages, the contrasting strains of the aggregate (expansion) and the cement matrix (drying shrinkage) initiate a distributed series of micro-cracks [2]. In addition, Spalling is caused by thermal strain and vapor pressure build-up in some situations, exposing deeper layers of concrete to burning and speeding up the heat transfer rate [3].

According to prior published studies [4, 5], the factors associated with the type of concrete have a significant correlation, and the type of material components impact the concrete compressive strength at high thermal conditions. Husem [6] researched how flexural and compressive resistance varied as high-performance concrete (HPC) and conventional Portland concrete (PC) were subjected to the heat of 200, 400, 600, 800, and 1000°C and subsequently cooled in water or air. The results show that (a) the compressive resistance of PC and HPC subjected to high thermal reading reduce as the temperature rises. The quick expansions that occur in the process of the deformation of mineral additive used in the HPC at high temperatures may cause the concrete to drop its strength. The results of the experiments showed that regular and high-performance concretes made with limestone aggregate lost a substantial amount of strength deprivation when chilled in freshwater since being subjected to extreme heat. Chan et al. [7] investigated the compressive and thermal behaviors of HPC at heating from 800 to 1100°C, and through the cooling process. It is discovered that followed by a gradual (26-34%) and quick (22-28%) cooling procedure, the strength attributes dropped dramatically. Tanyildizi et al [8] evaluated the

influence of high temperatures on featherweight concrete's tensile and compressive resistance using fly-ash. Temperatures of 200, 400, and 800°C were carried out in his study. Concrete's compressive and splitting tensile strength were reduced by 63.8% and 76.45%, respectively, at 800°C. Chan et al. [9] studied traditional and high-strength concrete put in high thermal conditions. The concrete compressive resistance at 28-day ages was measured after various temperature treatment durations (400,600, 800, 1000, and 1200°C). According to Tang et al., the concrete compressive strength using rubber-modified-recycled based aggregate was evaluated as rising heat [10].

It is evident that the compressive strength of concrete is affected by temperature variations, input material type, and mix proportions [1, 2, 11]. Typically, the statistical regression method estimates the concrete compressive strength at high thermal conditions based on laboratory test data. Although regression analysis appears to be easy and straightforward, the difficulty in the analysis increases as the number of independent variables grows [12]. More advanced techniques, such as Machine learning (ML), are used in complicated scenarios to improve model prediction accuracy. When considering the temperature changes, ML algorithms perform better and have a lower variance [11]. Some studies on predicting compressive strength of concrete based on ML models [13–22]. It can be seen that ANN is a commonly used model in research on strength prediction of concrete because its effectiveness in nonlinear modeling has been well demonstrated, and its mathematical background is clear [23]. Hocine et al [24] predicted the compressive strength of concrete using limestone powder by applying the ANN model based on 7 input variables related to the proportions and age. The results show that the correlation coefficient (R^2) of all training, testing, and validation phases is very high (over 97%). In addition, Behfarnia et al [25]. used ANN and adaptive neural-based fuzzy inference (ANFIS) to predict the compressive strength of

conventional concrete (without using admixtures or additives such as fly ash, silica fume, blast furnace slag, etc.) based on 160 samples and 7 input parameters related to proportions. The results show that although both ANFIS and ANN show strong predictive power, ANN has better performance. Several studies [13–16] show that ANN is a very effective model for predicting the compressive strength of self-compacting concrete. Like other ML methods, ANN can suffer from an overfitting problem (especially with too small data but too high model complexity) [26]. The regularization in the ANN allows reducing error for obtaining the highest coefficient of correlation and lowest total square errors [27]. A tuning regularization technique in ANN that has been used very effectively is Bayesian regularization which has been used to successfully study various problems such as stock price prediction, data mining, etc [28–32]. Pre-distribution of model parameters and management of large weights are some of the Bayesian regularization strategies used for ANNs to obtain smoother mapping [33].

Currently, there is no evaluation of the ANN-based Bayesian regularization model's effectiveness in predicting the strength of concrete as subjected to high temperatures. So, the development of this ML model to predict compressive strength and performance comparison was evaluated as part of this study's novelty. Temperature and material composition, including water, cement, coarse aggregate, fine aggregate, nano-silica, fly ash, super-plasticizer, and silica fume, were the 9 input parameters considered and used to evaluate the efficacy of the developed ANN technique in predicting concrete compressive strength.

2. Database construction

This paper develops an ANN model based on Bayesian regularization based on 208 experimental data to forecast concrete's compressive strength. The factors affecting the compressive strength of concrete such as the content of ingredient material in the designed

concrete mixture, including water, cement, aggregate (coarse sand/fine), mineral additives (silica-fume, nano-silica, fly ash), chemical additives (super-plasticizers), and subjected temperature have all been demonstrated in previous studies [34–39]. The statistical information of the input and output parameters is shown in Table 1. The input variables are denoted by I1 to I9, and the output parameter is denoted by O.

Fig 1 shows correlation matrix analysis, which visualizes the relationship between variables and analyzes each variable's effect on the problem's output variable. Different colors describe the correlation values. The blue square represents the negative correlation, and the red color represents the positive correlation. The pairs of attributes with a high degree of correlation can be removed to reduce the influence of unnecessary variables on the predictive model. The correlations between the inputs and output are not strictly linear, with a maximum correlation value of about 0.5. So, all inputs are considered as independent variables, while output as a dependent variable is predicted based on these independent ones.

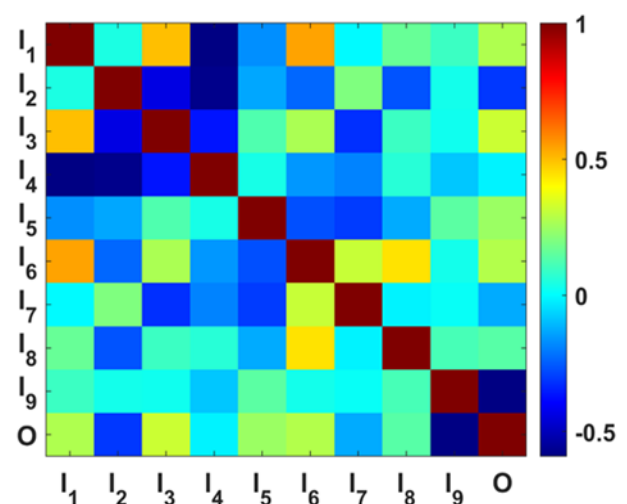


Fig 1. The distribution chart and correlation between inputs and output in this work

The dataset is divided into two groups for training and testing phases with a ratio of 70:30 to build the model. Finally, statistical parameters

and K-fold cross-validation validate the generated model.

Table 1. Statistical analysis of the input parameters in this study

Calculate for 1m³ concrete

Parameters	Abbreviation	Unit*	Min	Max	Mean	StD
Inputs						
Cement	I_1	kg	250	786	437.69	95.49
Water	I_2	kg	123	385	182.75	59.95
Fine Aggregate	I_3	kg	0	1345	610.13	317.39
Coarse Aggregate	I_4	kg	0	1681	1052.13	309.41
Fly Ash	I_5	kg	0	150	12.65	33.07
Super Plasticizer	I_6	kg	0	25.9	8.58	7.60
Silica Fume	I_7	kg	0	150	29.32	37.09
Nano Silica	I_8	kg	0	22.5	1.74	5.25
Temperature	I_9	(°C)	20	1000	354.52	287.65
Output						
Compressive strength	O	(MPa)	3	133.6	49.31	25.17

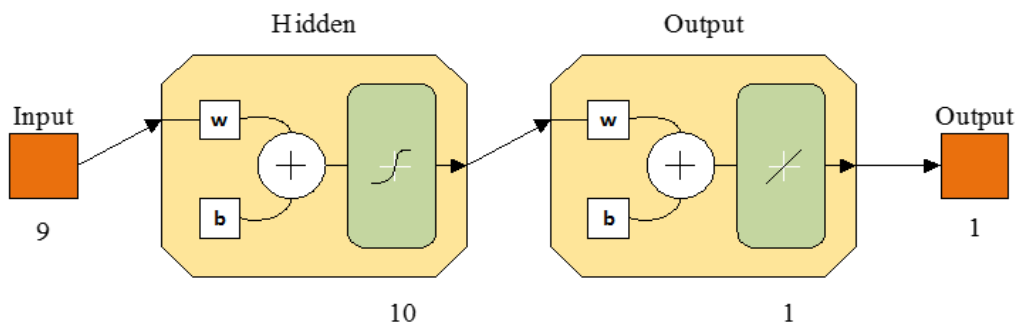


Fig 2. The structure of ANN in this study

3. Model Details

3.1. ANN

Artificial Neural Networks (ANN) have been introduced since the 1940s [23]. ANN is a strong machine learning-based data analysis technique that is based on actual biological neural networks and is used to analyze large amounts of data. This ML technique aims to imitate the knowledge acquisition and inference processes in the human brain to improve performance [40]. The use of artificial neural networks (ANNs) to handle nonlinear regression analysis issues has become more and more popular.

The ANN is set up to work based on biological neurons. A set of neurons is arranged so that all neurons receive an input signal and output signal simultaneously, and such a set is called a network layer [41]. The most straightforward neural network consists of a layer specializing in receiving input signals and input variables (input layer), and the output layer releasing the output signals. Hidden layers are those that exist between the input and output layers. These hidden layers contain hidden neurons, i.e., the intermediate results of the neural network's output value computation process. A neural network can have many hidden

layers. If there are too many hidden layers, the model will fit the data well, which also means that the model will be more accurate in estimating the weights but will be less accurate in predicting out-of-sample measurements [42]. In addition, the larger the number of hidden layers, the greater the number of weights in the model thereby making the model estimation time longer [43]. The structure of an ANN model in this study is shown on Fig. 2.

The use of Bayesian regularization in artificial neural network training/learning is much more potent than the standard back-propagation algorithm since it decreases or removes the requirement of extensive cross-validation [44]. In the same way, the regression method makes a non-linear model into a "well-posture" statistic issue, Bayesian regularization does the same for a nonlinear regression [33]. As a result, the models are reliable, and the assessment procedure is the advantage of Bayesian regularized-based artificial neural networks.

In statistics, the Bayesian approach differs from the probability perspective in hypothesis validating. It is founded on a couple of basic concepts: (1) probability is a metric of confidence of the events occurring, (2) past assumptions affect subsequent assumptions. The Bayes theorem states that [45]:

$$P(H|D) = \frac{P(D|H)P(H)}{P(D)} = \frac{P(D,H)}{\int_H P(D,H')dH'} \quad (1)$$

$$P(D) = \int_H P(D,H')dH' \quad (2)$$

The equation also holds in the probability approach, in which H and D are regarded groups of outcome measures. H is a hypothesis regarding if it has some previous assumption, and D is information that will modify one's assumption about H, according to the Bayesian approach. The probability is defined as $P(D|H)$. It represents the model's unpredictability (aleatoric-uncertainty), i.e., the controversial question or uncertainty by process noise in the model. The

prior is $P(H)$ and Eq (2) is subsequent. The posterior is defined as $P(H|D)$.

To put it another way, the Bayesian theory provides a good framework for quantifying uncertainties in ML techniques. Also, it gives an accurate basis for interpreting several of the regularization methods and training tactics utilized in traditional ML [46].

3.2. K-Fold cross-validation

When it comes to estimating the performance of machine learning models, cross-validation is the statistical approach utilized. It is often used to compare and select the most appropriate model for a given situation. Compared to previous approaches, this strategy is simple to grasp and use, providing more reliable estimations [47]. The most critical parameter to consider when using this strategy is K, which specifies the number of groups into which the data will be divided. It is referred to as K-fold cross-validation as a result of this. When a value of K is chosen, that value is used directly in the name of the evaluation method. This technique usually includes the following steps [48]:

- Shuffle the dataset at random
- Divide dataset into K groups. For each group: (i) Use the current group to evaluate model effectiveness; (ii) The remaining groups are used to train the model; (iii) Train the model; (iv) Evaluate and then reject the model
- Synthesize the effectiveness of the model based on the evaluation data

The total results are usually the average of the evaluations. In addition, the addition of variance and standard deviation information to the total results is also used in practice [49]. On the other hand, if K is chosen too large, the training set will be much larger than the testing set, and the evaluation results will not reflect the true nature of the machine learning method, especially with large data sets. That is also the reason why the 10-fold cross-validation is chosen

by many researchers [11, 48]. Therefore, in this study, K=10 was selected (10-fold cross-validation).

3.3. Performance assessment

The proposed ANN model's performance is evaluated using several indicators, comprising mean absolute error (MAE), root mean square error (RMSE), mean squared error (MSE), mean absolute percentage error (MAPE), and coefficient of determination (R^2).

The following equations reflect these values [43]:

$$R^2 = 1 - \left[\frac{\sum_{i=1}^n (P_i - E_i)^2}{\sum_{i=1}^n (P_i)^2} \right] \quad (3)$$

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (P_i - E_i)^2} \quad (4)$$

$$MAE = \frac{1}{n} \sum_{i=1}^n |P_i - E_i| \quad (5)$$

$$MAPE = \frac{100\%}{n} \sum_{i=1}^n \left| \frac{E_i - P_i}{E_i} \right| \quad (6)$$

Where E is the actual experimental value, P denotes the expected value based on the model's estimate, and n denotes the total sample sizes in the dataset.

R^2 is an important criterion in regression analysis. It is understood as the square of the correlation coefficient between the predicted outcome and the target, varying from 0 to 1. A high R^2 value indicates a good correlation between the predicted and the actual values. RMSE is an error measurement of the mean squared difference between the predicted and actual outputs of an ANN network model, while MAE measures the mean absolute error between them. Moreover, MAPE reflects how much the predicted value differs from the mean value. In contrast to R^2 , lower RMSE, MAE, MAPE values indicate better performance of the AI algorithm. All the criteria are necessary to evaluate the network model [50].

4. Results and Discussion

In the case of ANN training, the effectiveness of the model is determined by the topology of the neural network, which includes the number of hidden layers and the number of neurons in each of the hidden layers. Many factors that influence the ANN's performance, including the network's number of input and output parameters, the number of data points in the dataset, the training algorithm, the complexity of the error function, the network architecture, and the noise in the target data. A hidden layer in an ANN architecture, on the other hand, has been proven in several experiments to be sufficient for reaching the model's best performance [12, 40]. To this end, three layers in the proposed ANN structure were used to predict the compressive strength of concrete at high temperatures in this investigation. The input layer consisted of 9 neurons corresponding to 9 input parameters, the output layer consisted of 1 neuron representing the compressive strength value, and there was a single hidden layer between the two layers. It was necessary to experiment with different numbers of neurons in the hidden layer to establish the appropriate number of neurons in the hidden layer. Following multiple trial and error experiments, it was discovered that 10 neurons in the hidden layer produced the best prediction results in this study. These findings are derived from the training and validation results obtained after 10-fold cross-validation. Figure 3 shows the results of 10-fold cross-validation for a variety of assessment metrics. After 10 iterations, the R^2 measures from the training set are higher than those from the testing set, and the values of error (RMSE, MAE, and MAPE) from the training set are lower than those from the testing set, which clearly indicates the model's accuracy in predicting the compressive strength of concrete.

The regression model showing the correlation results between the predicted value from the ANN model and the actual value for the training and testing datasets is shown in Fig. 4. These are the typical prediction results from Fig. 3 (results of the Cross-Validation 2), in which the

horizontal axis represents the results of the collected experiment, and the vertical axis represents the results predicted by the developed ANN model. It is observed that the values obtained from the constructed ANN model for the training data set (Fig. 4a) and the testing dataset (Fig. 4b) are very close to the experimental results. In addition, the performance metrics are RMSE=2.757, MAE=2.004, $R^2=0.988$, and MAPE=5.387, whereas RMSE=6.159, MAE=4.438, $R^2=0.942$, and MAPE=14.164 for the test phase. These results show that the ANN model can generalize input and output parameters and provide good predictions. Also seen is that the linear regression lines are quite close to the diagonals, confirming the strong correlation between the anticipated and real compressive strengths. In this study, it is discovered that the produced ANN model can accurately predict the compressive strength of concrete when exposed to high temperatures.

Fig 5a shows the ANN model's distribution plot and cumulative distribution line of error for the training phase, while Fig. 5b shows those for the testing phase. It can be seen that the errors in both phases are concentrated around the 0 MPa position with a high density. In addition, based on the cumulative distribution, about 95% of the errors are concentrated in the very close range of 0 MPa, which confirms the modeling ability simulates the compressive strength of concrete accurately. Only a few cases with high errors (10 MPa, 20 MPa) were detected in the training and testing part, respectively. However, it does not affect the generalizability of the above machine learning model.

In this next section, the strength prediction result obtained from a multi-variable regression formulation is conducted (Eq. 7).

$$O = 19.047 + 0.095(I_1) - 0.050(I_2) + 0.003(I_3) + 0.007(I_4) + 0.339(I_5) + 0.506(I_6) + 0.015(I_7) + 0.518(I_8) - 0.061(I_9) \quad (7)$$

For the sake of comparison, the same training dataset was used to train the regression

model, whereas the same testing data set was used to evaluate the performance of the proposed formulation. Fig. 6a shows the results of statistical indices, the ideal regression line, and the model's fit line for the training set. The values of statistical indices for the training part, including high R^2 value (0.974), and low error (RMSE=4.085, MAE=2.733, and MAPE=8.016) indicated the high accuracy of the proposed formulation. The fit line nearly coincides with the ideal regression line, which confirms the close correlation between predicted and actual compressive strength. Nevertheless, Fig. 6b shows the formulation results on the testing dataset. It can be seen that there is a very significant difference between the ideal regression line and the fit line in the linear regression, showing the model's insufficient accuracy. In addition, $R^2 = 0.718$, RMSE=13.334, MAE=10.838, and MAPE=34.315 are much lower than the predicted results from the model on the training data set.

Finally, the results of this study are compared with those of Ahmad's study using Decision Tree (DT), Artificial neural network (ANN), Bagging, and Gradient Boosting (GB) models proposed in [11]. As shown in Table 2, it can be seen that the proposed ANN-based Bayesian regularization model in this paper has better predictive performance (the highest R^2 , and the lowest errors RMSE and MAE) than the other models. This result is also similar to some previous publications. Artificial neural network-based Bayesian regularization performed better than Partial Least Squares Discriminant Analysis (PLSDA) in chemical and drug metabolism prediction [51]. As compared with some algorithms to improve ANN efficiency, Bayesian regularization shows superiority over Levenberg–Marquardt algorithm [26, 52] and gradient descent with momentum and adaptive learning rate backpropagation – GDX [53], Scaled Conjugate Gradient (SCG) [54]. Besides, Gouravarajua [27] concludes that the artificial neural network-based Bayesian regularization combined with the K-fold cross-section technique

which can greatly reduce computation time with high accuracy can be used to successfully study gecko adhesion problems. Thus, it is shown that utilizing the ANN-based Bayesian regularization

model to estimate the compressive strength of concrete at high temperatures is achievable, hence saving time and money on trials.

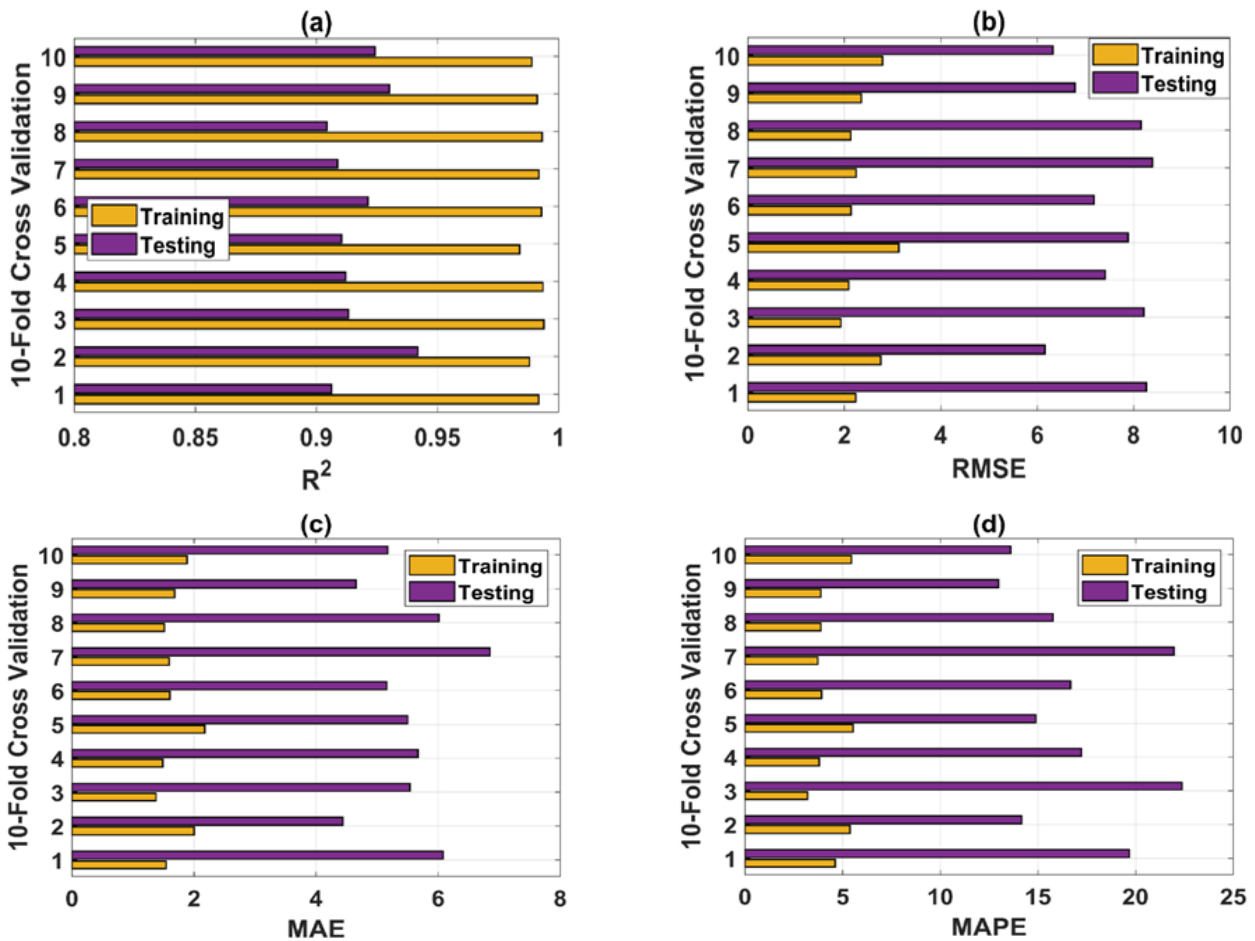


Fig 3. Results of training and validation of ANN model after 10-fold cross-validation based on different performance evaluation criteria: (a) R^2 ; (b) RMSE; (c) MAE, (d) MAPE

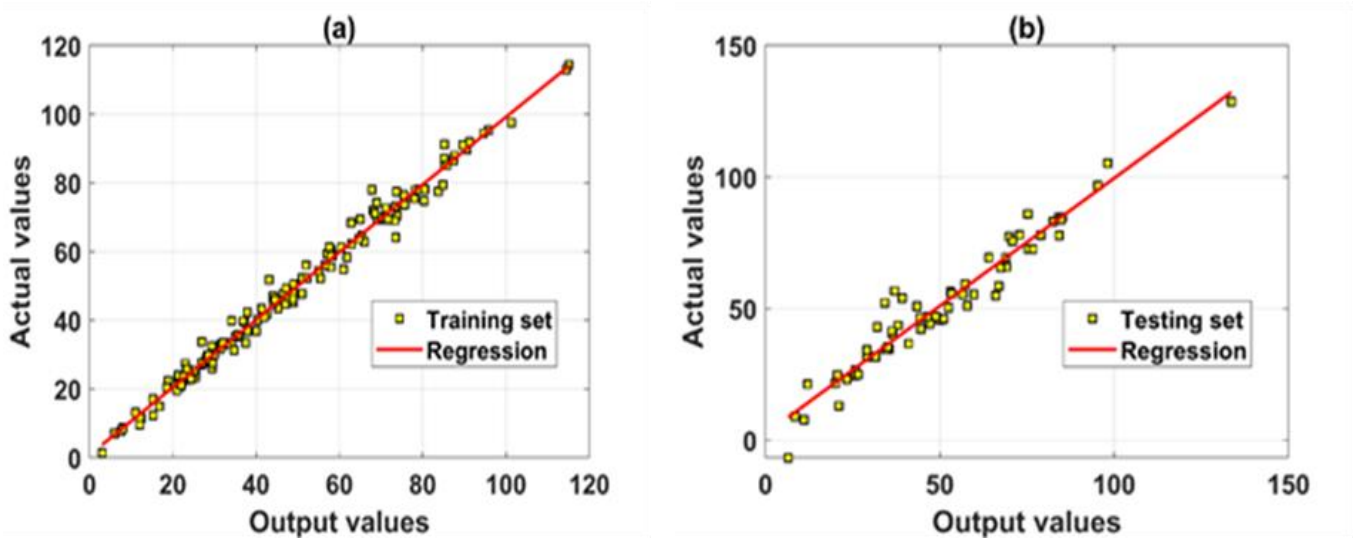


Fig 4. Comparison of the performance of ANN model with the actual values for the (a) training dataset and (b) testing dataset

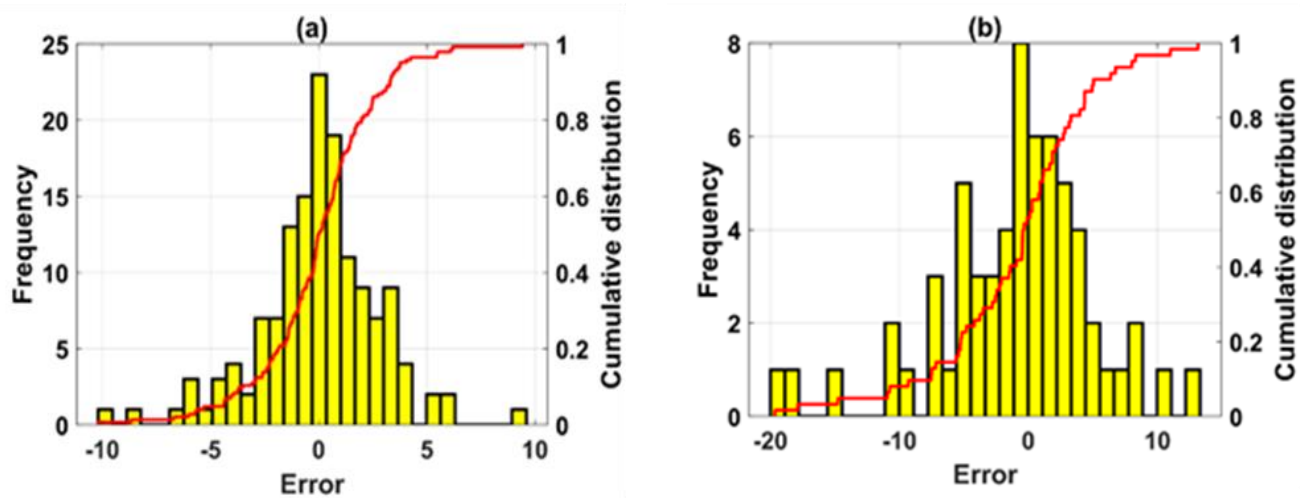


Fig 5. Error and regression charts between experimental values and simulation values calculated by ANN considered in this study for: (a) the training part; and (b) testing part

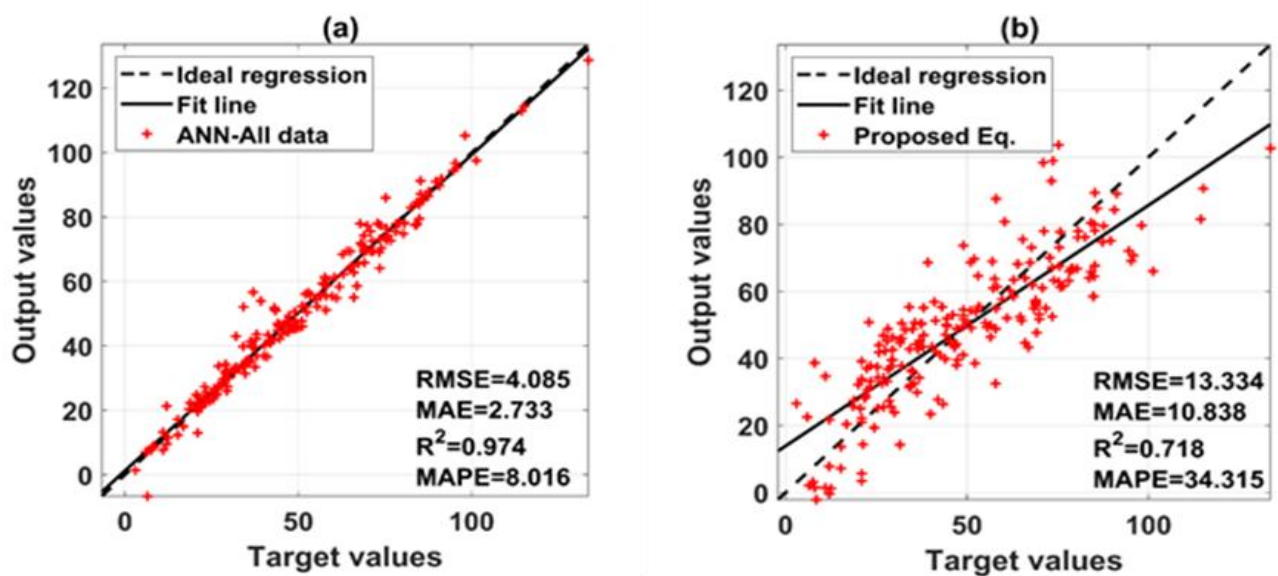


Fig 6. Regression graphs showing a comparison between the experimental values and the predicted results obtained by formulation Eq. (7)

Table 2. Comparison of the prediction results

	ML model	R^2	RMSE	MAE
This study	ANN -Bayesian regularization (Training)	0.988	2.757	2.004
	ANN-Bayesian regularization (Testing)	0.942	6.159	4.438
Ahmad's study [11]	DT	0.8378	10.79	7.54
	Bagging	0.9047	7.81	5.65
	GB	0.8854	9.24	6.93
	ANN	0.8202	11.03	9.15

5. Conclusion

Based on Bayesian regularization, an optimum neural network is presented to forecast the compressive strength of 28-day concrete at high temperatures. A total of 208 experimental results were collected from experimental results used to construct the ANN-based Bayesian regularization model. Water, cement, coarse aggregate, fine aggregate, nano-silica, fly ash, super-plasticizer, silica fume, and temperature were all included in the input space of the collected database. Four statistical criteria were used to evaluate the performance of the model. The prediction accuracy is $R^2=0.942$, $RMSE=6.159$, $MAE=4.438$, and $MAPE=14.164$. The suggested ANN model's performance in this research was compared to that of the previous study and found to be superior. Concrete's compressive strength under various temperature settings may be accurately predicted using the ANN model, saving time and money otherwise spent on costly experiments. ML hybrid models might need to be developed based on this preliminary study to improve the accuracy of estimating concrete's compressive strength at high temperatures.

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