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Concrete compressive strength prediction by artificial neural network approach

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Abstract

The structural integrity of concrete structure is explicitly influenced by concrete compressive strength (CS). Timely prediction of concrete compressive strength exhibits good performance in the field of construction. However, it is very challenging due to the unpredictable physical and mechanical properties of concrete and its constituent ingredients. To mitigate the limitation of the laboratory testing-based experimental method, this manuscript presents optimal artificial neural network (ANN) model to forecast CS. For this purpose, total number of 776 datasets were collected from previous research papers. The preprocess dataset was randomly split into training and testing sets. After that, optimal ANN model was developed by establishing appropriate hyperparameters with random search method. The over-fitting and validation loss were stabilized by loss function assessment with Adaptive optimization algorithms (Adam) optimizer. The output results of the optimized ANN model exhibit good prediction performance with R-squared value of 0.87, and errors such as MAE, MSE, and RMSE with values of 3.419 MPa, 21.909 MPa, and 4.68 MPa, respectively. In addition, SHAP value of the output model shows volume of cement and time have highest positive impact, whereas water and fly have highest negative impact on concrete compressive strength. This paper shows the power of machine learning techniques to timely and efficient prediction of concrete compressive strength. Thus, this optimal ANN model is applicable in concrete made infrastructure design and construction industry.

Keywords: *Artificial neural network; compressive strength; loss function; prediction; SHAP.*

1. Introduction

In the construction field, concrete remains a critical material worldwide due to its strength, flexibility, and relatively low cost. It is a composite material primarily composed of cement, water, fine and coarse aggregates, and sometimes admixtures. The physical and mechanical properties of these ingredients significantly affect concrete's compressive strength, quality, and durability. As a result, detailed impact assessments are crucial for improving the overall performance of concrete compressive (Chithra et al., 2016; Prabhu et al., 2014; Katuwal, 2019a; Parashar et al., 2020; KC et al., 2022; Singh & Siddique, 2012). In structural design, the overall performance of structural components is explicitly influenced by concrete compressive strength. In addition, the structural durability and strength of concrete composite structures are highly influenced by concrete compressive strength, which is vital for determining linear or nonlinear modeling parameters in structural design (Banjara et al., 2021; Bhusal et al., 2020; Chaulagain et al., 2015; Ghimire & Chaulagain, 2021). Therefore, accurately determining concrete compressive strength is essential for enhancing the structural strength and durability of concrete-made infrastructures.

Traditionally, laboratory testing methods and empirical equations have been used to determine concrete compressive strength (Prabhu et al., 2014; Singh & Siddique, 2012). These methods show good results; however, undesirable results can be seen due to unpredictable physical and mechanical properties of concrete ingredients. Moreover, these methods are very challenging, time-consuming, and costly. To address these limitations, robust artificial intelligence prediction models have emerged as useful tools for forecasting concrete compressive strength.

In recent decades, many researchers have applied machine learning algorithms for classification and regression analysis in the civil engineering field (Bhattarai et al., 2022; Gautam et al., 2024; Katuwal et al., 2024; Pyakurel et al., 2023). These studies have demonstrated the strong prediction capabilities of machine learning algorithms. Specifically, several researchers have employed machine learning (ML) techniques to forecast concrete compressive strength (Chithra et al., 2016; Chopra et al., 2014; Mahajan & Bhagat, 2022; Paudel et al., 2023; Song et al., 2021; Song et al., 2022; Thapa, 2024a; Thapa, 2024b). Some researchers applied the artificial neural networks (ANN) method to determine concrete compressive strength (Bu et al., 2021; Chithra et al., 2016; Khademi et al., 2016; Topçu & Saridemir, 2008). These machine learning algorithms and artificial neural network methods show good prediction performance and have a strong correlation between predicted and actual concrete compressive strength.

However, previous studies have limitations, such as relying on data from specific sources or laboratory tests and using simple ML algorithms or ANN methods with limited input datasets. To address these gaps, this research proposes an optimal artificial neural network (ANN) method by aggregating 776 data points from various previous studies conducted in different laboratories. This approach not only bridges the gap between conventional laboratory methods and advanced ANN techniques but also aims to optimize different ANN hyper-parameters for predicting concrete compressive strength.

The novelty of this study lies in its comprehensive data collection and optimization of ANN hyperparameters, which have not been extensively explored in existing literature. The performance and reliability of the proposed model were evaluated using the loss function (MSE), several statistical indices, and SHAP values, demonstrating its superior prediction accuracy and robustness compared to existing methods.

2. Artificial Neural Network

The artificial neural network (ANN) algorithm was inspired and evolved by simulating the ideas with the function and structure of biological neural networks in the human brain (Jain et al., 1996). Hence, the working methodology of ANN is more or less similar to working function of human brain. The fundamental function of each artificial neuron is to receive information from input features, process it, and outputs are transferred into the next layer of neurons. Neurons consist of two parameters such as weight and bias, and act as basic processing units of neural networks. During the training phase, these two parameters are learned from the input and adjusted weights based on the error of the output is compared to the expected result. ANN consists of input layer and, output layer, and these layers may or may not be connected with number of hidden layers. The input layer has many nodes which depends on the number of input features.

This input layer receives the preprocessed data and transfers it into hidden layers of the neural network. The real processing is performed in hidden layers through a system of weighted connections. Thus, hidden layer optimization is often essential to increase the performance of neural networks. Consequently, the output layer provides the final result as a response of artificial neural networks to input features. In ANN, the feed-forward neural network is a straightforward model, where input data is processed in a single direction from input to output, which means it does not have back-propagation. This network may or may not have hidden layers (Raschka & Mirjalili, 2019).

The overall function of the artificial neural network has been established by the function of weight, input, and bias from input to output. In addition, in ANN, the basic operation of neurons is obtained by using the following equation to determine the output of each layer.

$Z = \Phi\,(i.W+b)$ .... (1)

Where, input features are represented by i, and weight matrix is represented by W and bias vector for each layer is indicated by b. In addition, the Φ represents the activation function. Similarly, Z is a pre-activation vector that represents the output of each input layer transferring statistics from one layer to the next layers. This transformation is both linear (through weights and biases), and non-linear (through activation function). Thus, it enables ANN to effectively train the model even with complex relationships. The choice of activation function significantly depends on types of specific data and characteristics of the problem. The following equations are widely used activation functions.

Sigmoid (Logistic Function) $\Phi = \frac{1}{1+e^{-z}}$ .... (2)

Hyperbolic Tangent Function (Tanh) $\Phi = \frac{e^{z}-e^{-z}}{e^{z}+e^{-z}}$ .... (3)

Rectified Linear Unit Function (ReLU) $\Phi = \max(0, z)$ .... (4)

The ANN learning algorithms enable to tuning iteration between weight and bias in each neuron with the use of activation function and show good mapping from input to output. However, certain errors occurred during the forward propagation, hence, this error is updated in the neural network by propagating errors backward from output to input layer with application of algorithms called back-propagation (BP). The main objective of BP is to minimize error function by adjusting the weights and biases of neural network is called loss function. Hence, back-propagation is often used in the field of artificial neural networks (Werbos, 1990). In this ANN model, two main steps are involved. Firstly, forward propagation is performed in each network layer to compute the loss between predicted output and actual output by using loss function. After that, the backward pass was conducted from output layer to the input layer via hidden layers to update the weights and biases of network using appropriate optimization algorithms like gradient descent and adaptive optimization algorithms. This process is continuously repeated with multiple epochs until the stopping criterion is met. The effectiveness of BP depends on the choice of activation function, number of hidden layers, learning rate, and optimization algorithms used for back-propagation. Hence, optimal parameter selection is essential to increase the performance of the ANN model.

3. Model Development

In this research, concrete compressive strength and its ingredients-related data were collected from previous research (Aggarwal & Siddique, 2014; Agudelo et al., 2022; Basar & Deveci, 2012; Bilal et al., 2019; Prabhu et al., 2014; Guney et al., 2010; Katuwal, 2018; Katuwal, 2019b, Mahajan & Bhagat, 2022; Manoharan et al., 2018; Mavroulidou & Lawrence, 2019; Parashar et al., 2020; Siddique et al., 2018; Singh & Siddique, 2012; Song et al., 2021; Song et al., 2022; Thiruvenkitam et al., 2020). A total of 776 number of data were preprocessed with cleaning, correlation analysis, and data distribution. These preprocessed datasets were split into training set (80%) and test set (20%). After data splitting, the min-max normalization technique was used to make a uniform scale for all selected parameters. The optimal ANN model was selected and trained with training dataset. After that, trained model was tested with test set. The performance of ANN model was evaluated by using different statistical parameters, which are discussed in following section. Hyper-parameter tuning was applied if ANN model output results were not within the desired range. Conversely, if the predictive outcomes meet expectations, these results are compared and the final regression model was established for prediction. The detailed research methodology employed in this study for ANN regression analysis is illustrated in Figure 1. In addition, a comprehensive discussion is conducted in the following subsection.

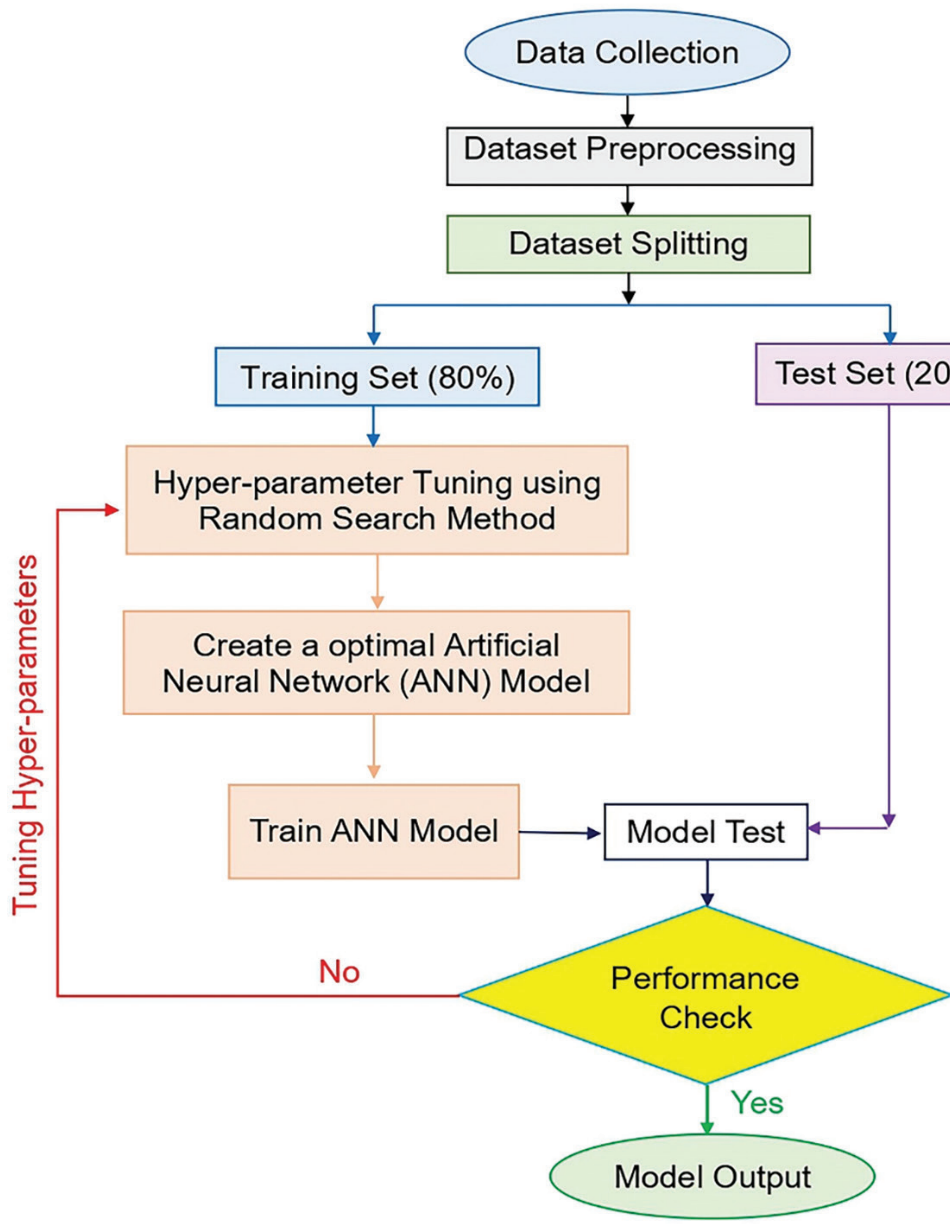

Figure 1: Working methodology flowchart

Table 1 demonstrates the statistical details of selected dataset. Table 1 breaks down these parameters into their different values such as mean, standard deviation, minimum value, maximum value, and occurrence of different percentile like 25%, 50%, and 75%. This Table 1 shows the dimensions and scale of selected input parameters and target variable. In this research, the concrete compressive strength (CS) was selected as target variable which depends on different ingredients such as cement (C), water (W), sand (S), coarse aggregate (CA), fly ash (FA), curing time (T), and super-plasticizer (SP), which were selected as input features.

Table 1: Statistics of the selected features

Parameters	Mean	Std	Min	25%	50%	75%	Max
Cement (C)	300.2	98.27	134.7	218.9	290.1	372	540
Water (W)	182.1	17.96	140	168.2	186	192.9	238.6
Sand (S)	765.7	148.1	0	734.9	780.5	830	1820
Coarse aggregate (CA)	1026.9	142.4	410	966	1028.4	1086.8	1385.2
Fine aggregate (FA)	69.6	63.54	0	0	97	124.8	200.1
Super-plasticizer (SP)	4.6	5.33	0	0	3.7	9.4	28.2
Time (T)	31.4	27	1	14	28	28	100
Concrete compressive strength (CS)	30.9	13.4	6.27	20.4	29.8	39.8	79.9

3.1 Data preprocessing

In machine learning (ML), data preprocessing is the foremost and very crucial step for transferring raw data into the required format of ML algorithms. This technique handles missing values, cleans or removes any noise, scales features, encodes features, selects the appropriate feature, and finally transfers the selected dataset into a suitable format of ML algorithms. In this research, Pearson's correlation coefficient was used to evaluate correlation between selected parameters. This correlation is plotted in a heat map and presented in Figure 2. This process presents a detailed description of how two or more variables are correlated to each other. This method is helpful to identify the appropriate input variables, which means not correlated parameters should be excluded from selected datasets. Figure 2 presents a detailed description of correlations between selected parameters. This heat map shows a coefficient within the range of -1 to +1. The higher positive value indicates that these parameters are highly correlated and vice versa. The coefficient value zero represents no correlation between variables.

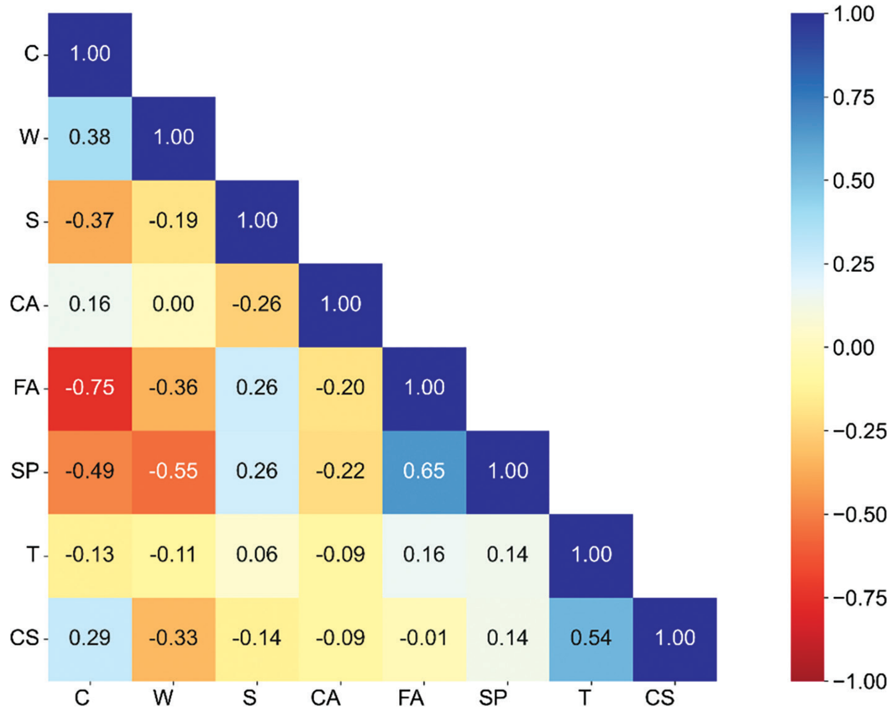

Figure 2: Pearson's correlation coefficient between selected parameters with heat map

Figure 2 shows that concrete compressive strength has a high positive correlation with curing time (T) with value of 0.54, and volume of cement (C) with value of 0.29. This means these variables have a high positive influence on concrete compressive strength (CS). In contrast, amount of water (W) has negatively correlated with concrete compressive strength with value of 0.33. In addition, the Figure 2 illustrates that concrete compressive strength is negatively correlated with amount of sand, coarse aggregate, and fine aggregate with values of 0.14, 0.09, and 0.01, respectively. Thus, these selected parameters have a considerable effect on the determination of concrete compressive strength. Thus, these all parameters are selected as input variables for further regression analysis.

3.2 Data distribution

Data distribution involves examining and visualizing selected parameters to understand their patterns, characteristics, and statistical structures. Figure 3 shows how data points are spread out across different values in the combined form of a histogram and kernel density estimation (KDE) plot. In addition, the histogram in this figure illustrates a graphical representation of frequency distribution of each input feature and target variable, which means that it divides selected data into bins by exhibiting the number of specific observations that fall into each bin. For example, target variable (CS) varies from 6.27 to 79.9 MPa, and the median value of 29.88 MPa. Thus, this plot demonstrates the numerical data distribution in other input features as well.

The probability density function of random variables is evaluated by using KDE as shown in Figure 3, which demonstrates the pattern of underlying data. The concrete compressive strength (CS), cement (C), and sand (S) follow a normal distribution with a single peak point i.e. it shows unimodal distribution. The fly ash (FA) curve follows a normal distribution with two distinct peaks, i.e. it follows a bimodal distribution. Moreover, other plots in water (W), coarse aggregates (CA), super-plasticizer (SP), and curing time (T) have no clear normal distribution and these plots exhibit multiple peaks. In conclusion, this combination of histogram with KDE curve exhibits a good understanding of the shape and structures of data distribution in selected input features and target variable.

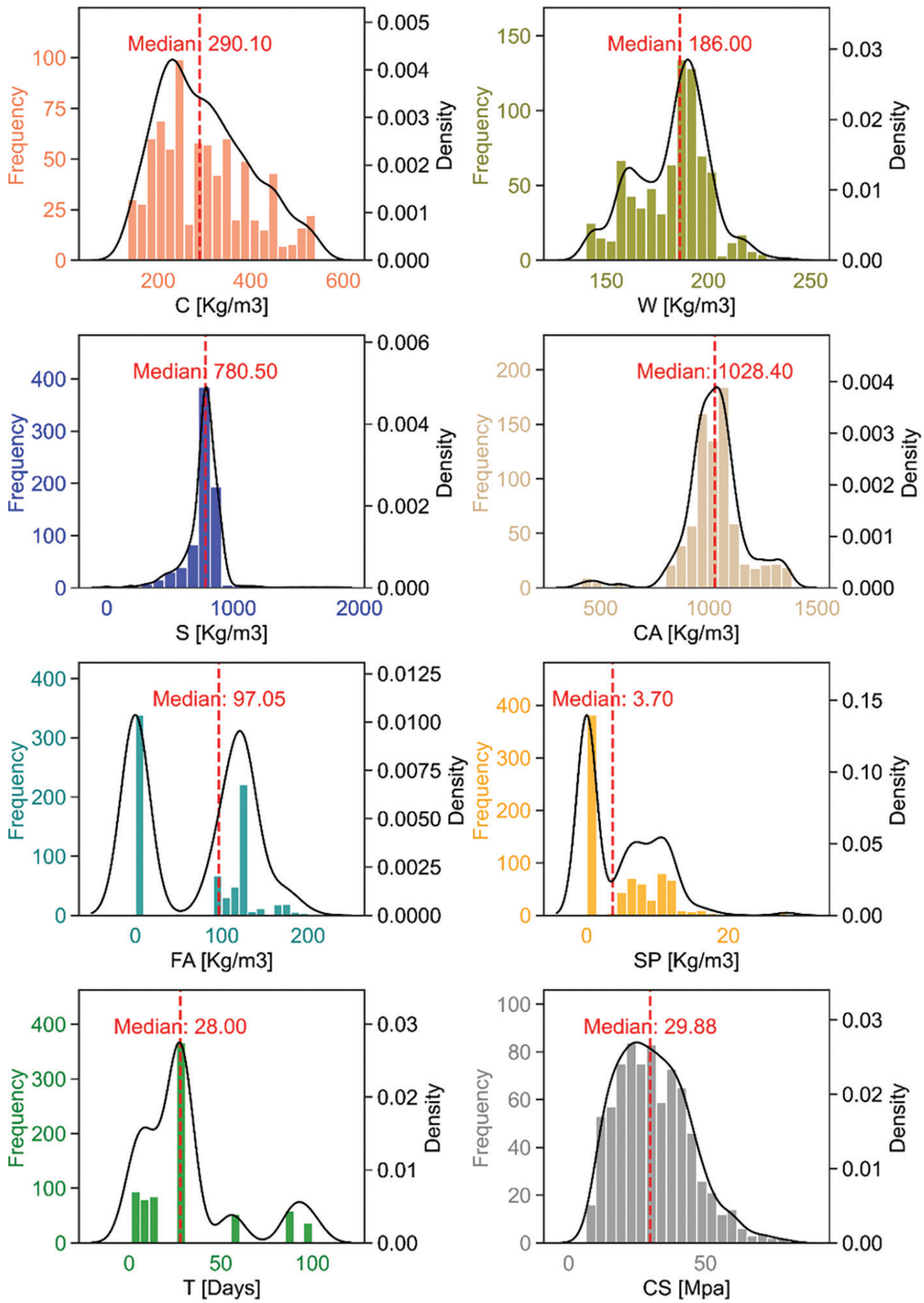

Figure 3: Histograms and corresponding kernel density estimate (KDE) plots

3.3 Data rescaling

The collected data sets for this study (presented in Table 1) are in different scales for input variables and target variable. Therefore, it is essential to rescale these parameters to ensure their consistency. Moreover, rescaling ensures that input feature values are in the same range and transferring selected data to the appropriate format of ML algorithms. Thus, this technique significantly influences the performance of models. For this purpose, min-max normalization was employed in this research to achieve a consistent scale across all parameters. This method scales all features within the range of 0 – 1. For rescaling of input features, following calculation formula was used.

$$X_n = (X - X_{min}) / (X_{max} - X_{min})$$

In this formula, X denotes the actual value of the parameters, while X_n represents the normalized values. The maximum and minimum values of the input features are represented by X_{max} and X_{min}, respectively.

3.4 ANN model development with optimal hyper-parameters

In this ANN model, two main steps are involved: forward and backward propagations. In forward propagation, preprocessed input features such as cement (C), water (W), sand (S), coarse aggregate (CA), fly ash (FA), super-plasticizer (SP), and curing time (T) were selected in the input layer. After processing of ANN regression model, a random search method was applied to establish different optimal hyper-parameters. The obtained optimal results are presented in Table 2. These optimal hyper-parameters significantly reduce model overfitting or underfitting and improve ANN model interpretability, optimize the resource utilization, and eventually enhance model prediction performance.

Table 2: Optimal hyper-parameters for artificial neural network

Hyper-parameters	Value
Output layers	Number of features = 7,
First hidden layer	Neurons = 352, activation function = tanh, kernel_initializer = 'he_normal'
Second hidden layer	Neurons = 480, activation function = relu, kernel_initializer = 'he_normal'
Output layer	Neurons = 1, activation function = linear
Optimal number of epoch	72
Batch size	32
Optimizer	Adaptive optimization algorithms (Adam)
Loss function	mean_squared_error

Based on these optimal values, two hidden layers were established between input and output layers with optimal parameters, which are presented in Figure 4. After that, final prediction was determined in output layers. These output results were compared with actual value and computed the loss function of neural networks. The minimum loss function represents better prediction performance of ANN model. However, some errors exist between predicted and actual values. Thus, appropriate algorithms are essential to minimize this loss function via the back-propagation process.

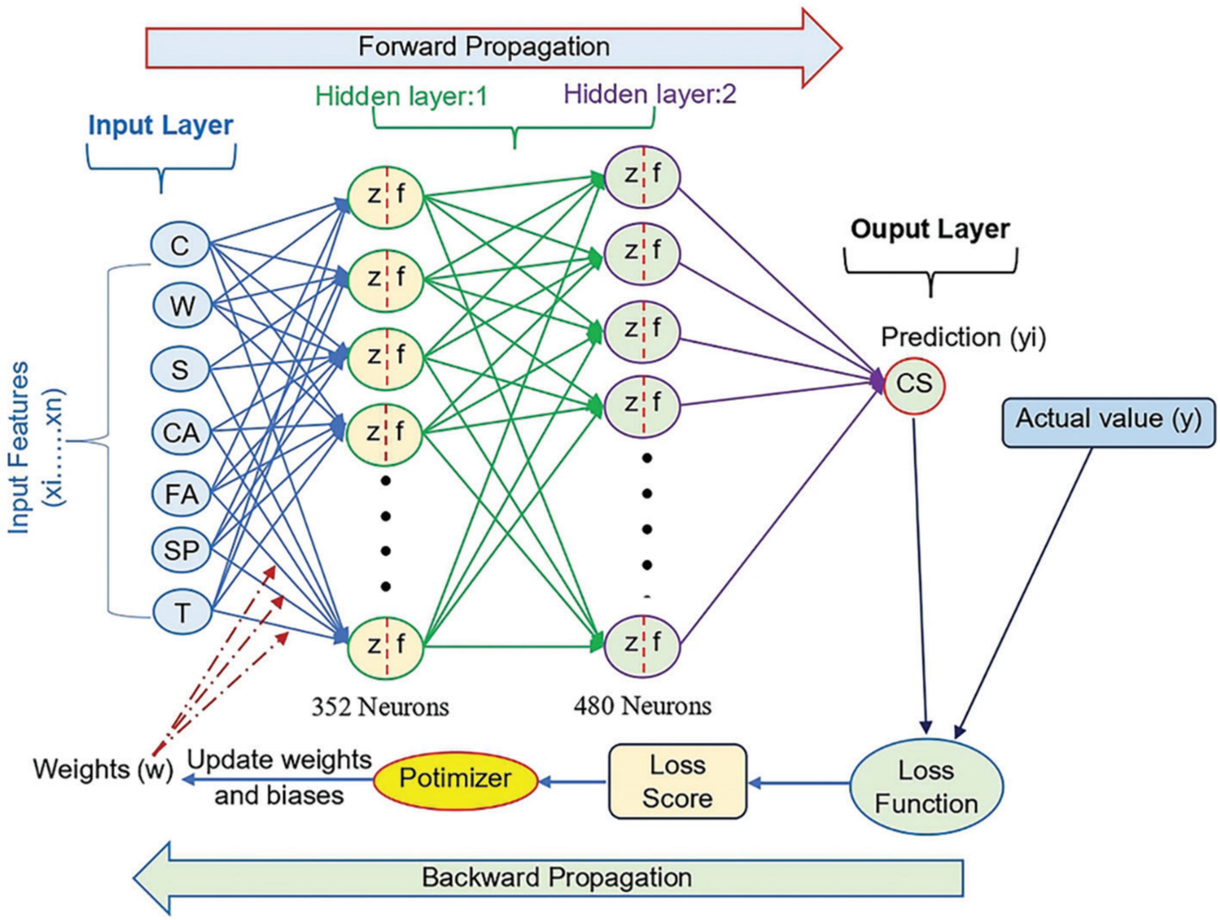

Figure 4: Artificial neural network (ANN) model diagram

In this research, the chain rule was used to determine the loss score, and Adaptive optimization algorithm (Adam) was used to compute the gradients of loss function concerning weights and bias in neural networks. This forward, loss calculation, backward propagation, and parameter adjustments were conducted with an iterative process until a defined number of epochs or convergence criteria were met. Thus, the effectiveness of ANN regression model is significantly controlled by its hyper-parameters.

3.5 Performance evaluation statistical indicators

The effectiveness of regression model is typically assessed through various statistical metrics to evaluate the performance and verification of selected model. Thus, these metrics are essential to determine accuracy and efficiency of predictive models. In this study, equations (5) to (12) were utilized to evaluate the performance of artificial neural network (ANN) model.

R-squared (R2) = $\frac{\text{sum of squared regression (SSR)}}{\text{sum of squared total (SST)}}$ ....(5)

Mean absolute error (MAE) = $\frac{1}{n}\sum_{i=1}^{n}\left|y_i^a - y_i^p\right|$ ....(6)

Mean squared error (MSE) $\frac{1}{n}\sum_{i=1}^{n}\left(y_i^a - y_i^p\right)^2$ ....(7)

Root mean squared error (RMSE) = $\sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(y_i^a - y_i^p\right)^2}$ ....(8)

Relative root mean squared error (RRMSE)= $\sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(\frac{y_i^a - y_i^p}{y_i^a}\right)^2}$ ....(9)

Mean absolute percentage error (MAPE) = $\frac{1}{n}\sum_{i=1}^{n}\left|\frac{y_i^a - y_i^p}{y_i^a}\right| * 100\%$ ....(10)

Mean relative error (MRE) = $\frac{1}{n}\sum_{i=1}^{n}\left|\frac{y_i^a - y_i^p}{y_i^a}\right|$ .... (11)

Variance accounted for (VAF) = $1 - \left|\frac{\text{va}\,(y_i^a - y_i^p)}{\text{var}(y_i^a)}\right| * 100\%$... (12)

In this equation, y_i^a indicates actual values of selected parameters, y_i^p indicates the corresponding regression model predicted values, and 'n' denotes the total number of data used in training or testing stages.

3.6 Shapely additive explanations

In machine learning, the contribution of selected input features in output performance of target variable is evaluated by using a unified framework like Shapley Additive Explanations (SHAP). The SHAP value of each input feature shows its impact on the output performance and illustrates a clear understanding of how each selected input feature impacts the target variables (Lundberg & Lee, 2017). Thus, this SHAP value shows the contribution of input features with the corresponding ranking for a specific task.

4. Results and Discussion

4.1 Loss function validation

Loss function evaluation in training and validation sets against epochs is essential for effective model training, generalization assessment, and model selection. This evaluation is useful for model overfitting detection and selection of optimal parameters in artificial neural network regression model. Figure 5 illustrates the loss function of training and validation sets against number of epochs. In Figure 5, both training and validation losses drastically decrease at the beginning and slightly decrease after epoch of 15. This initial steep decrease indicated that both training and validation begin to learn from a randomly initialized state. After the 15th epoch, both curves decrease gradually in a smooth curve that indicates that the artificial neural network (ANN) model has a less pronounced rate of decrease losses, which means improvement slows down.

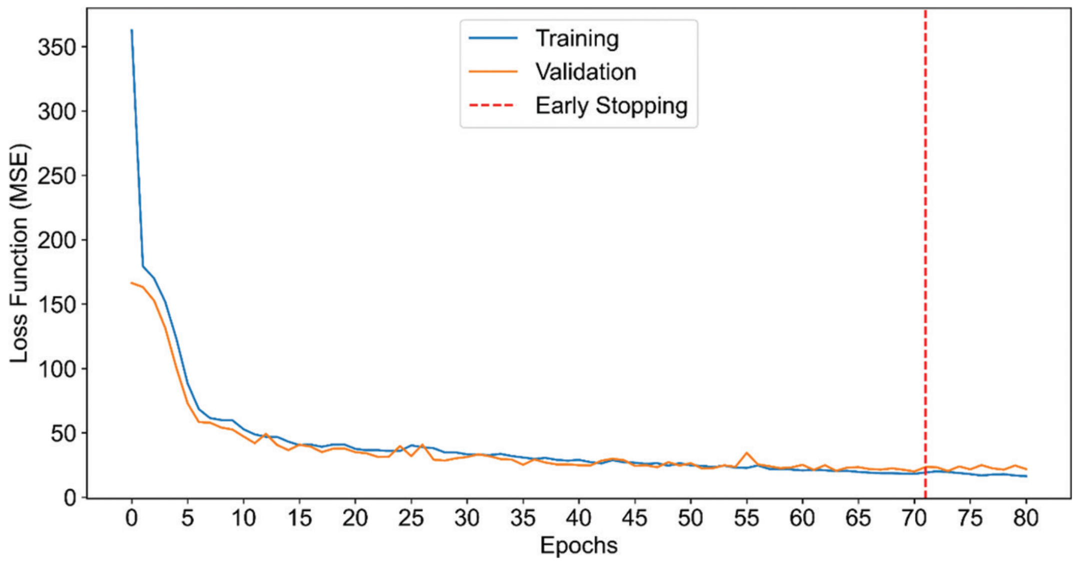

Figure 5: Loss function of training and validation sets against epoch

In Figure 5, the early stopping line with the epoch of 72 indicates that the training process performs well and yields minimum validation loss. In addition, the Figure 5 shows that the training process stopped at the epoch of 72. These results indicated that in the last 8 epochs (80-72), validation loss starts to increase and is higher than the training loss, which increases overfitting in artificial neural networks model. Thus, for this ANN model, 72 epoch numbers were selected to prevent overfitting conditions.

4.2 Artificial neural network regression model

In this study, the preprocessed train set data was trained with optimal hyper-parameters, which are illustrated in Table 2. The trained ANN model was tested with preprocessed test set data. This ANN model shows excellent statistical indicators and good prediction performance. The output result of the ANN model is presented in Figure 6.

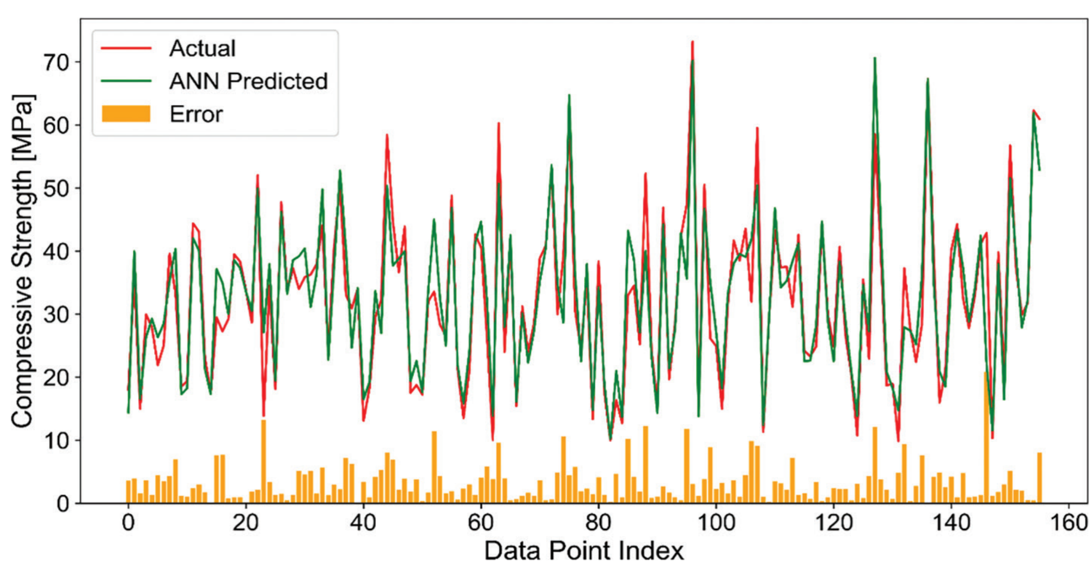

Figure 6: Distribution of actual and predicted concrete compressive strength with errors

Figure 6 illustrates the distribution of concrete compressive strength predicted value with actual value. Also, the Figure 6 illustrates the errors measured in the prediction model with corresponding data points. Ae correlation between the actually measured and ANN model predicted concrete compressive strength is presented in Figure 7. The Figure 7 shows that good correlation with R-squared value of 0.87 and Pearson's r value of 0.93. These values show that the ANN model has good prediction performance.

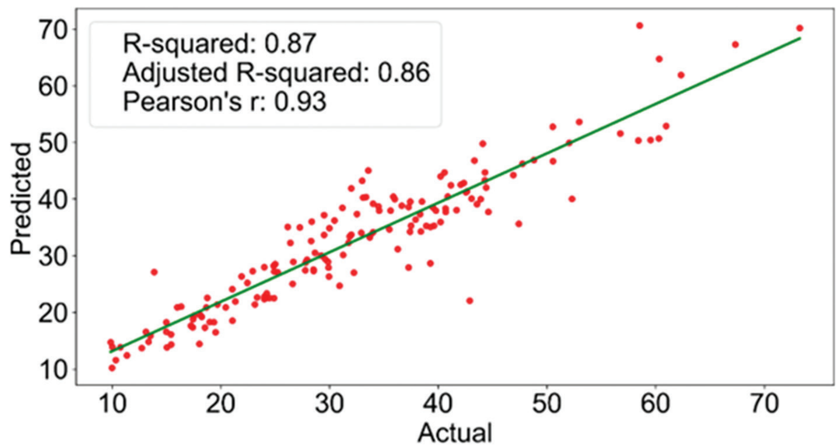

Figure 7: Correlation between predicted versus actual results

The statistical indicators of this ANN model are presented in Table 3. The R-squared value and VAF of ANN model are 0.87, and 86.91%, respectively. These results exhibit the ANN model has good prediction performance. In addition, the MAE and MSE values of this ANN model are 3.419 and 21.909. Other statical indicators presented in Table 3 show that the use of optimal hyper-parameters in the ANN model significantly improves the prediction capabilities of this regression model.

Table 3: Statistical indicators of the artificial neural network (ANN) model

Indicators	R^2	VAF	MAE	MRE	MSE	RMSE	RRMSE	MAPE
Values	0.87	86.91%	3.419	-3.588%	21.909	4.68	0.145%	11.622%

4.3 Features importance analysis

The SHAP value method was used to describe the importance of each feature and its impact on the target variable. This method originates from cooperative game theory and calculates the contribution of each feature to target variables. Figure 8 depicts the importance of selected input features to target concrete compressive strength. The cement (C) and curing period (T) have the highest positive impact on concrete compressive strength. In contrast, water has highest negative impact. In addition, fly ash (FA) has least positive impact, and coarse aggregate (CA), super-plasticizer (SP), and sand (S) have a negative impact on the prediction of concrete compressive strength using the ANN model.

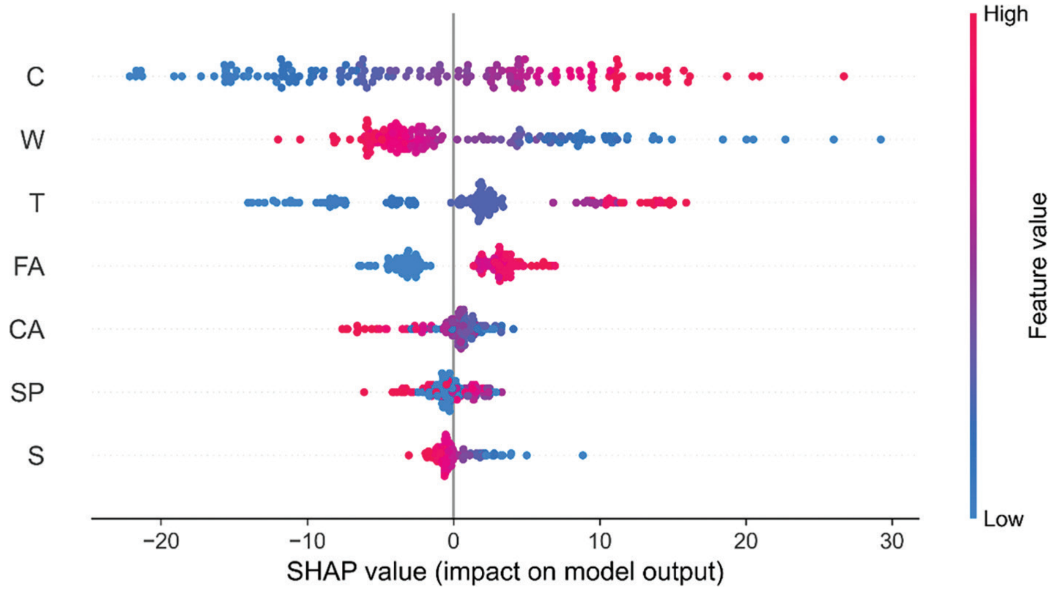

Figure 8: Features importance analysis using SHAP value method

5. Conclusions

In this research, 776 number of concrete compressive strength datasets were collected from previously published research papers. This research included different constituents of concrete with increasing sources of data to enhance the prediction of concrete compressive strength. These datasets were evaluated using artificial neural network (ANN) model with optimal hyper-parameters. This optimized ANN model was tested with test datasets and shows a good prediction performance to predict concrete compressive strength as indicated by various statistical indicators. Loss function in this ANN model exhibits valuable information about early stopping stage, mitigation condition for over-fitting, and validation loss stabilization stage. This research depicted that the epoch of 72 is suitable to prevent over-fitting and the last 8 epoch shows suitability for validation loss stabilization. Furthermore, it shows that the cement and curing time have positive impact on compressive strength of concrete, whereas water and fly ash have negative impact. The optimized ANN model can be applicable to predict concrete compressive strength with good performance, which contributes to advancement in timely prediction of concrete strength and facilitates novelty in material design and its utilization in concrete made infrastructures. Thus, this model can be used in real construction sites and further research.

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