Utilising Artificial Neural Networks for Prediction of Properties of Geopolymer Concrete

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Abstract. The most popular building material, concrete, is intrinsically linked to the advancement of humanity. Due to the ever-increasing complexity of cementitious systems, concrete formulation for desired qualities remains a difficult undertaking despite conceptual and methodological advancement in the field of concrete science. Recognising the significant pollution caused by the traditional cement industry, construction of civil engineering structures has been carried out successfully using Geopolymer Concrete (GPC), also known as High Performance Concrete (HPC). These are concretes formed by the reaction of inorganic materials with a high content of Silicon and Aluminium (Pozzolans) with alkalis to achieve cementitious properties. These supplementary cementitious materials include Ground Granulated Blast Furnace Slag (GGBFS), a waste material generated in the steel manufacturing industry; Fly Ash, which is a fine waste product produced by coal-fired power stations and Silica Fume, a by-product of producing silicon metal or ferrosilicon alloys. This result demonstrated that GPC/HPC can be utilised as a substitute for traditional Portland cement-based concrete, resulting in improvements in concrete properties in addition to environmental and economic benefits. This study explores utilising experimental data to train artificial neural networks, which are then used to determine the effect of supplementary cementitious material replacement, namely fly ash, Ground Granulated Blast Furnace Slag (GGBFS) and silica fume, on the compressive strength, tensile strength, and modulus of elasticity of concrete and to predict these values accordingly.

Keywords: Concrete, Artificial neural networks, Geopolymer concrete, High-performance concrete, Supplementary cementitious material, Fly Ash, Ground Granulated Blast Furnace Slag (GGBFS), Silica Fume, Reinforced concrete, Mechanical properties, Mortar.

1. Introduction

The construction industry is increasingly emphasising sustainability, and accordingly interest has increased sharply in recent years in developing environmentally friendly “Green Concrete” (Omran et al. 2014). Coal-fuelled power generation produces fly-ash as a primary waste material. Additionally, the waste product known as slag from steel and iron industries is widely available. Disposal of fly ash has proven to be costly and environmentally threating, whereas siliceous fly ash can be a valuable additive to concrete, resulting in green concretes with enhanced mechanical properties (Golewski 2018). In light of this, Supplementary Cementitious Materials (SCMs) are increasingly employed in concrete mixtures to enhance the properties of plastic and hardened concrete, typically by pozzolanic reaction. Examples of such materials include fly ashes, Ground Granulated Blast Furnace Slag (GGBFS), and silica fume (Far & Far 2018).

Adding these constituents to concrete mixtures enhances their mechanical and material properties by increasing strength, workability, resistance to fire and chemical attack and reducing permeability. In addition, using SCMs reduces cost, since these materials are recycled materials and by-products of other industrial processes (Duxson et al. 2007). Concretes incorporating Supplementary Cementitious Materials are referred to in the literature as Geopolymers (Davidovits 1991). Utilising SCMs correspondingly reduces the energy requirement of manufacturing cement and concrete, thus incurring further cost savings. Moreover, Supplementary Cementitious Materials are typically industrial waste materials which, if not utilised, would end up in landfills or man-made ponds where their contents are liable to leach into surface and ground water, causing extensive pollution and health hazards.

Geopolymer Concrete (GPC) has been found to have higher compressive strength than comparable concretes utilising ordinary Portland cement (Deb et al. 2015; Far & Flint 2017). Highlighting these enhanced properties, the phrase "High Performance Concrete" (HPC) has emerged as synonym for GPC in the construction sector. Geopolymer-based high performance and ultra-high performance concretes are accordingly considered some

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of the most promising materials for concrete construction (Abellán-García 2022). In addition to the Portland cement, fine and coarse aggregates, and water that make up traditional concrete, additional cementitious elements including fly ash and Ground Granulated Blast Furnace Slag (GGBFS) as well as chemical admixtures like superplasticiser are required for the production of Geopolymer and High Performance concretes; thus modelling the behaviour of these types concrete is a challenging endeavour due to the materials' extreme complexity (Yeh 1998).

Concrete mix design is a complex and important subject that necessitates expert knowledge of the consistent materials and challenges related to their use. Constructing a useful end-product, a building or bridge for example, is contingent on availability of concrete with the necessary strength and other utility qualities. Concrete hardening and hydration are irreversible processes. Therefore, any mistakes in the concrete mix design are quite expensive for the investor, both during construction and after the structure has been used due to reduced durability (Saleh et al. 2018; Tabatabaiefar 2016; Ziolkowski et al. 2019).

Facing these challenges, Artificial Intelligence (AI) is increasingly utilised in concrete research as a complementary approach, and is providing new perspectives and useful solutions for accelerating innovations in the design and development of cementitious materials. The intrinsic complexity of concrete mixtures and their attributes can be taken into account by (AI) by utilising current datasets with data-driven models, which can automatically learn implicit patterns. An experiment series employing a particular material is used to train a neural network, which is the fundamental approach to creating a brain-based model for material behaviour. The trained neural network will have enough knowledge of the material's behaviour to qualify as a material model if the experimental findings contain the pertinent information about the material's behaviour. Such a trained neural network should be able to approximate the outcomes of other trials in addition to being able to replicate the experimental findings it was trained on (Ghaboussi et al. 1991).

Machine learning and Artificial Neural Networks (ANN) have been employed in numerous studies to determine and predict the mechanical properties of concrete. Yeh (1998) prepared several batches of high performance concrete which showed satisfactory experimental results, and subsequently utilised the data to train an artificial neural network, concluding "the strength model based on the artificial neural network is more accurate than the model based on regression analysis". Chou et al. (2014) used advanced Machine Learning (ML) techniques to predict concrete compressive strength, concluding that their results confirm the suitability of ML methods for quick and effective concrete compressive strength computations. Getahun et al. (2018) employed an artificial neural network based modelling approach to predict the compressive and tensile strengths of concretes employing recycled construction and agricultural waste materials, finding that their model successfully predicted compressive and tensile strengths with only a 3% deviation from experimental results.

Reflecting the rapid increase in research in this area in recent years, Boğa et al. (2013) developed a four-layered artificial neural network method (ANN) and determined that the ANN model can estimate experimental data to a remarkably close degree. Dao et al. (2019) proposed AI algorithms and developed ANN models to predict the compressive strength of Geopolymer concretes incorporating Ground Granulated Blast Furnace Slag (GGBFS), and evaluating the models performance using metrics such as the absolute mean error (MAE) and root mean square error (RMSE). Dao et al. (2019) found that their model was capable of predicting compressive strength of GPC with MAE = 1.989 MPa, RMSE = 2.423 MPa; concluding that the ANN model possessed a strong potential for predicting the compressive strength of GPC.

It is necessary to identify appropriate assessment measures to analyse the effectiveness of AI/ML models. The Correlation coefficient (R) measures the strength of association between variables by estimating the strength of the linear association between them. Its use as a performance metric is well documented in the literature (Smith 1986). Among the advantages of the correlation coefficient (R) are that it is fairly straightforward calculate and provides a logical measure of the strength of linear association in the data. In a comprehensive comparative study of performance metrics, Naser et al. (2021) pointed out that a coefficient $R > 0.8$ implies strong correlation, adding that R does not change by equal scaling, can be used in predicting material properties well with numeric data, points which are in agreement with our logic to use Correlation coefficient (R) as a performance indicator in the current study.

To provide a thorough picture of the error distribution, numerous metrics may occasionally be needed. The RMSE offers a benefit when the error distribution is anticipated to be Gaussian and there are sufficient samples (Chai et al. 2014). Naser et al. (2021) further noted the sensitivity of the RMSE to outliers as an advantage, which is applicable to the current study due to the likelihood of outliers in experimental data. Ultimately, while no single measure of error provides a complete and accurate representation of error, the RMSE is deemed suitable for the current study.

This study investigates the potential of utilising artificial neural networks (ANN) to determine the effect of replacement of ordinary Portland cement with supplementary cementitious materials (SCM), notably fly ash, Ground Granulated Blast Furnace Slag (GGBFS) and silica fume, on the mechanical properties of hardened concrete, including compressive strength, modulus of elasticity and tensile strength. The main advantages of using a neural network approach are that all of a material's behaviour can be represented in a single, cohesive environment provided by a neural network, and the neural network-based model is created directly from experimental data using the neural network's learning capabilities. This study will not discuss in detail the artificial neural network methodology because it has been covered in numerous papers and books. Section 2 of the following sections provides an explanation of the artificial neural network. The network used to predict the compressive strength of concrete is examined in Section 3. The model is examined in Section 4 along with a number of proportioning factors in order to track the HPC's strength behaviour. To validate the suggested strategy, experiments are used in Section 5. Sections 6 and 7 provide results and conclusions.

2. Architecture of Artificial Neural Networks

Artificial neural networks (ANN) are a class of massively parallel architecture that function in conjunction with highly networked artificial neurons to tackle complex problems (Seiffert 2002). The structure and operation of the biological neural network serve as the foundation for ANN architecture. The neurons of ANN are arranged in several layers, just like the neurons in the brain. A common type of neural network is the feed-forward neural network, which has three layers: an input layer for receiving outside data needed for pattern recognition, an output layer for providing the solution, and a hidden layer that acts as an intermediary layer between the other layers. Acyclic arcs connect the nearby neurons in the input layer to the output layer.

The ANN employs a training algorithm to learn the datasets, and contingent on the error rate between the target and actual output, updates the neuron weights (Sairamya et al. 2019). The back propagation algorithm is typically used by ANN as a training procedure to learn the datasets. Fig. 1 depicts the general architecture of an ANN. The vast majority of research utilises back-propagation neural networks (McClelland et al. 1987).

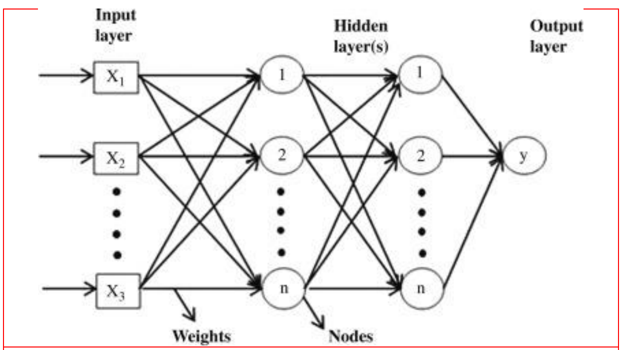

Fig. 1 General structure of an Artificial Neural Network (ANN) (Sairamya et al. 2019).

The network is trained by altering the link weights in accordance with the knowledge it has gained through training. By comparing each input pattern's goal output with the network's output for that pattern, the network learns by computing the error and propagating an error function backward through the network. After the network has been trained, it is given values for the project's input parameters in order to run. Following that, the network computes the node outputs using the weight values and thresholds already in place from the training phase. Because the system only needs to generate the network node values once, executing the network happens very quickly (Zupan 1994).

To test the accuracy of a trained network, the Root Mean Square Error (RMSE) is adopted, which is a commonly used method for comparing values predicted by a model or estimate to values observed in a sample or population. It gauges how well the proposed model can predict and replicate patterns in the experimental data in order to forecast the outcome (Hyndman et al. 2006).

3. Modelling of strength of Geopolymer concrete

3.1 Learning Algorithm

The Levenberg-Marquardt method has been used as the learning algorithm to train the ANN model for the current study (Marquardt 1963). The Gauss-Newton and Gradient Descent functions are both used by this approach to access the best run-by-run performance. While gradient descent uses the idea of absolute minima and absolute maxima, Gauss-Newton uses MSE as the cost function; the criterion which quantifies how good a model is (Sheskin 2004). By updating the parameters along the steepest-descent direction, the gradient descent method reduces the sum of the squared errors (Gavin 2020). The absolute maximum is the highest value on a cost function graph, whereas absolute minimum is the lowest point on the graph. Because it makes use of both the Gradient Decent and the cost function, the Levenberg-Marquardt algorithm performs better than other algorithms (Bafitlhile et al. 2018). Since this algorithm gets the optimal value more quickly than other algorithms, it requires less training time (Wilamowski et al. 2010).

The number of neurons in the Hidden Layer is determined as follows. The number of hidden layer neurons are 2/3 (or 70% to 90%) of the size of the input layer. If this is insufficient then number of output layer neurons can be added later on (Boger et al. 1997). The number of hidden layer neurons should be less than twice of the number of neurons in input layer (Berry et al. 2011).

With these considerations in mind, the cost function was optimised to determine the number of neurons in the hidden layer. The performance of the cost function was recorded for each iteration of the program, which was repeated a number of times. It was decided to choose the number of neurons that predicted the output with the highest correlation.

3.2 How the ANN code functions

The first step is importing the data set from the directory. Subsequently, pre-processing of the data (correlation, null values, filling missing data points) is carried out. Pertinent research has shown that when less than 10% of the cases had missing data, implementing imputation techniques were superior to dropping cases with missing values and performance of the downstream predictive process is significantly improved by imputation. (Jäger et al. 2021; Langkamp et al. 2010). Thus, filling null values and missing data points was conducting by sorting the data and averaging of the variable before and after the missing value, as per established methods, a procedure conducted for less than 10% of the data. This was followed by distinguishing of input and output variables. The authors appreciate this insightful comment from the reviewers. Data is split for training, validation, and testing in proportions of 80%, 10%, and 10%, respectively. This distribution has been found to achieve a high degree of training and validation accuracy (Golchubian et al. 2021). Chi et al. (2022) conducted a comparison between a 70-15-15 split and an 80-10-10 split, finding the latter to achieve a higher rate of training and validation accuracy and noting “the best way to increase model performance and reduce overfitting on the dataset side was to use an 80-10-10 split of the data”, obtaining training accuracy of 91.53% and validation accuracy of 97.11%. These results show that the 80-10-10 split is well established in the literature and has been shown to achieve high levels of accuracy. In addition, the dataset employed in the current study is class balanced, whereby random sampling is optimally suited.

Model construction is then carried out utilising 10 neurons. RMSE is subsequently calculated for every output, and the actual and anticipated values are used to produce the regression plot. This is followed by optimizing the quantity of neurons to produce the best correlation between experimental and predicted values. Optimisation allows for selecting the ideal number of neurons and reinforcing the model. Finally, the regression plots are replotted and the RMSE recalculated. The steps above are illustrated in the following flow chart shown in in Fig. 2.

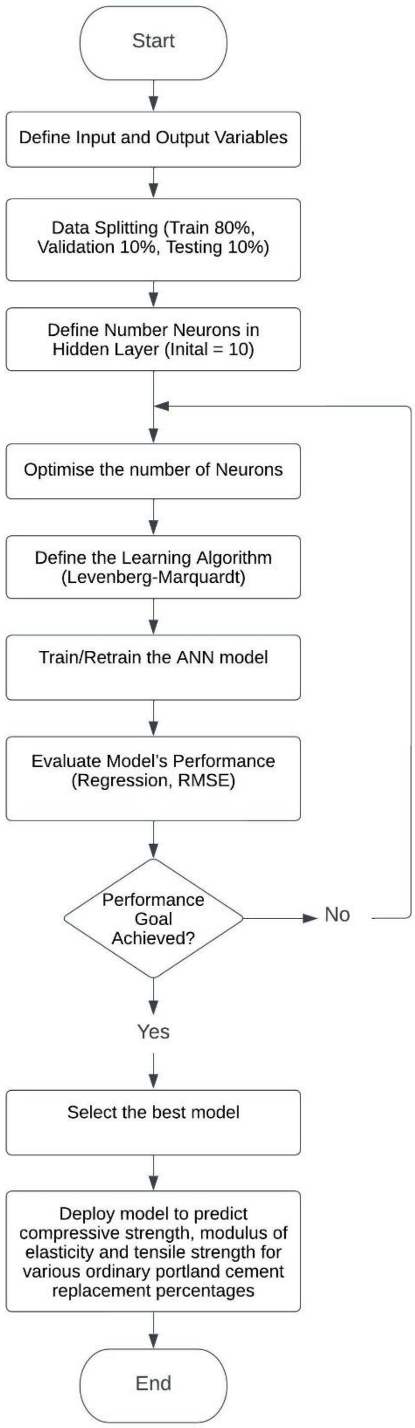

Fig. 2 Modelling methodology flowchart for current study

4. Modelling of strength of Geopolymer concrete

This study uses data obtained from the National Research and Development Project, known as New RC Project, supported by the Ministry of Construction and the

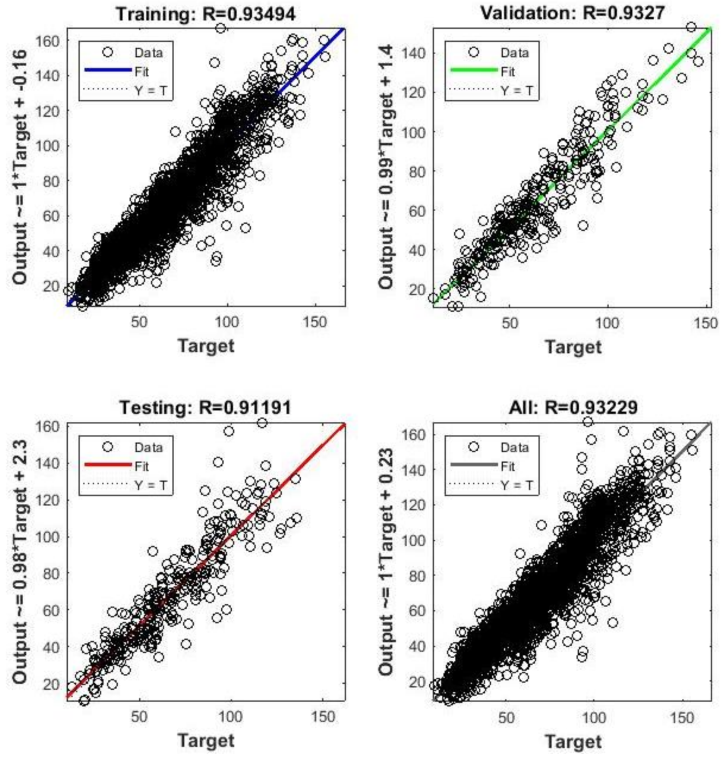

Fig. 3 Model performance: Predicted compressive strength values of neural network compared with values actually observed in the laboratory for the testing examples.

Research Committee on High-strength Concrete of the Architectural Institute of Japan (Tomosawa et al. 1995). More than 3,000 data points on the correlation between concrete composition and mechanical properties including compressive, tensile strengths and modulus of elasticity were gathered and statistically analysed (Tomosawa et al. 1995). These data points were gathered by numerous researchers using a variety of materials. The examined concretes' compressive strengths ranged from 20 to 160 MPa, with data collated and presented in Tomosawa et al. (1995). A total of 2903 data points were utilised in this study. A statistical analysis of this dataset is provided in Table 1.

Table 1 Statistical analysis of dataset of experimental values (Tomosawa et al. 1995)

	Performance Comparison in case of Compressive Strength		
	Compressive Strength (MPa)	Modulus of Elasticity (GPa)	Tensile Strength (MPa)
Mean	65.33	33.35	3.89
Median	60.60	34.30	3.77
Standard Deviation	28.88	8.62	1.33

This data is used to train the developed artificial neural network developed for this study, such that by varying the factors of fly ash content, Ground Granulated Blast Furnace Slag (GGBFS) content and silica fume content, predictions for the value of compressive strength, modulus of elasticity and tensile strength can be obtained.

5. Training Results

As stated in the earlier explanation of the ANN code and shown in Figure 2, splitting for training, validation, and testing in proportions of 80%, 10%, and 10%, respectively had been carried out. The training results can be summarised as follows.

5.1 Compressive Strength:

Initially the model was trained with 10 number of neurons in the hidden layer, and the predications for compressive strength obtained and compared to experimental results. The performance of the model can be observed in the regression plots shown in Fig. 3.

Fig. 3 shows the comparison between the predicted compressive strength and the actual values reported in the experimental results in Tomosawa et al. (1995). The sample correlation coefficient (R) measures how closely the points on a scatter plot are related to a linear regression line constructed using those points, with a value close to 1 indicating a strong correlation. Performance of the model is acceptable for training but may be improved in the case of testing, therefore an attempt is made to optimise the number of neurons. Fig. 4 illustrates the optimisation process.

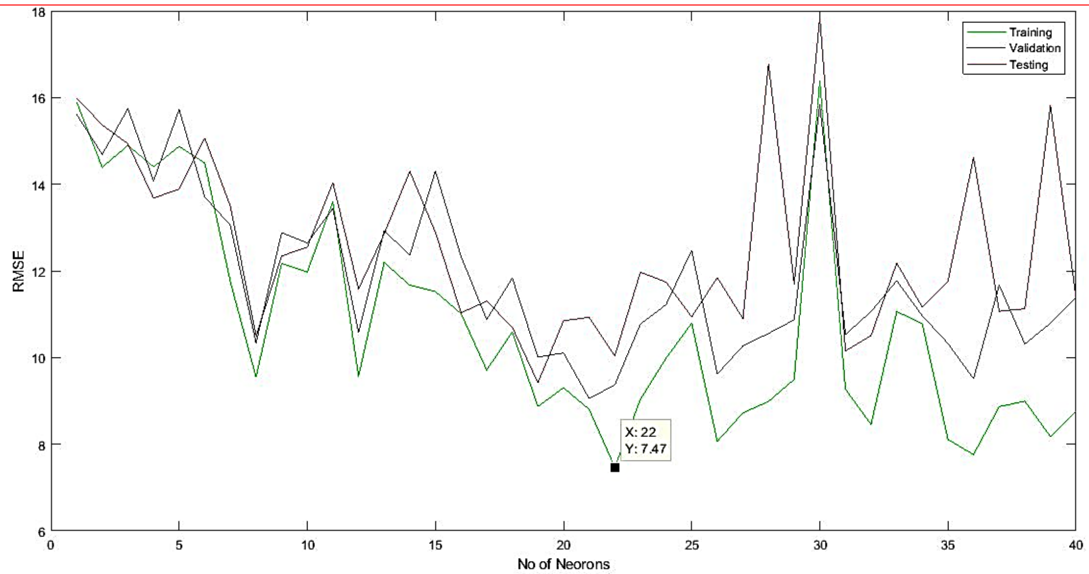

Fig. 4 Optimisation of the number of neurons adopted in the ANN for prediction of compressive strength.

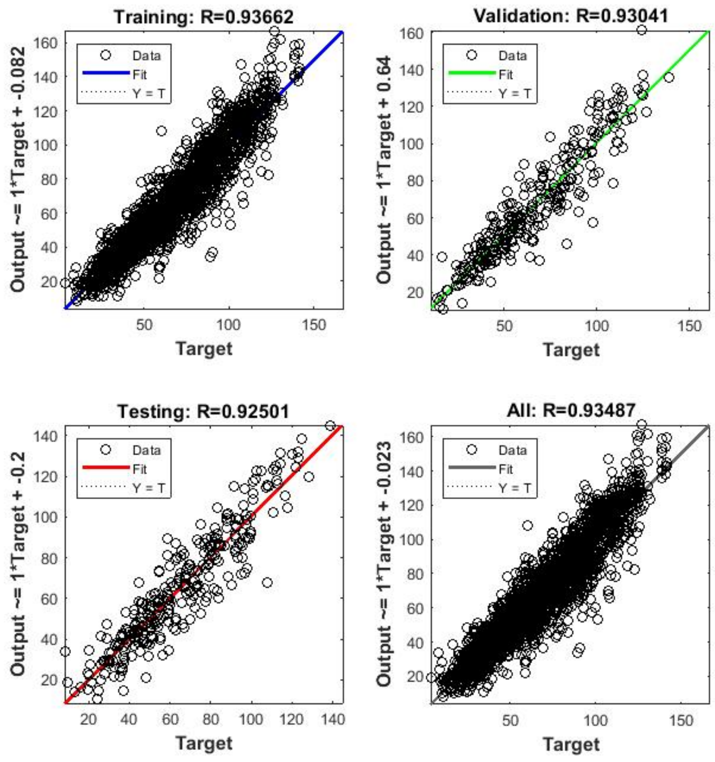

Fig. 5 Model performance: Predicted compressive strength values of neural network compared with values actually observed in the laboratory for the testing examples using optimized number of neurons.

Based upon the optimisation process shown in Fig. 4, the number of neurons adopted in the ANN is modified to 19, in order to minimise the RMSE. Using the optimised number of neurons and rerunning the analysis, the obtained predicted compressive strength values were as follows (Fig. 5).

The results are summarised in Table 2. These results show reduced root-mean-square error (RMSE) upon using the optimised number of neurons.

Table 2 Performance Comparison of RMSE for prediction Compressive Strength

Performance Comparison in case of Compressive Strength		
State	RMSE (10)	RMSE Optimised (19)
Training	12.367	8.969
Validation	11.213	11.177
Testing	13.730	9.816

5.2 Modulus of Elasticity:

Initially the model was trained with 10 number of neurons in the hidden layer, the performance of the model can be observed in the following regression plot (Fig. 6).

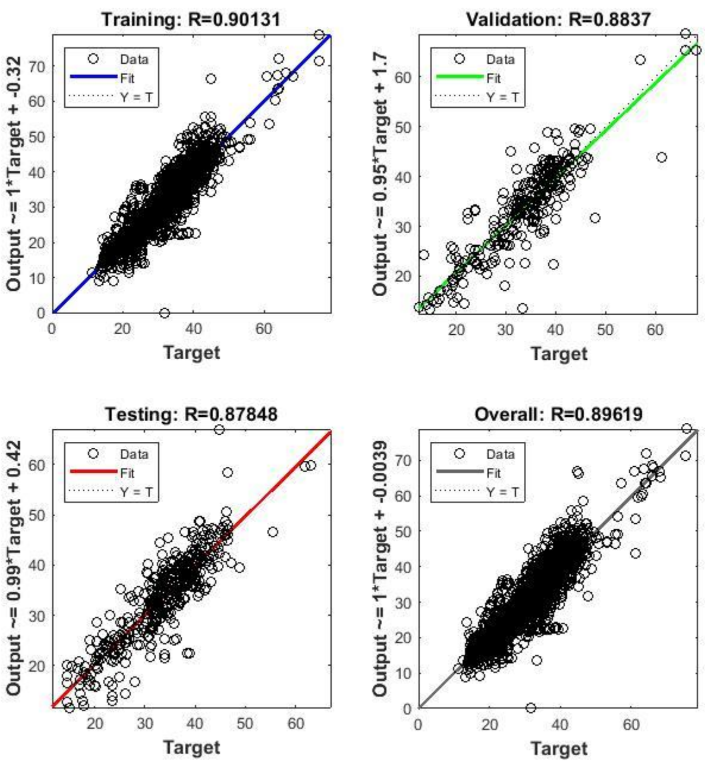

Fig. 6 Model performance: Predicted modulus of elasticity values of neural network compared with values actually observed in the laboratory for the testing examples using number of neurons (10).

The performance shown in Fig. 6 has been improved using the optimisation process shown in Fig. 7.

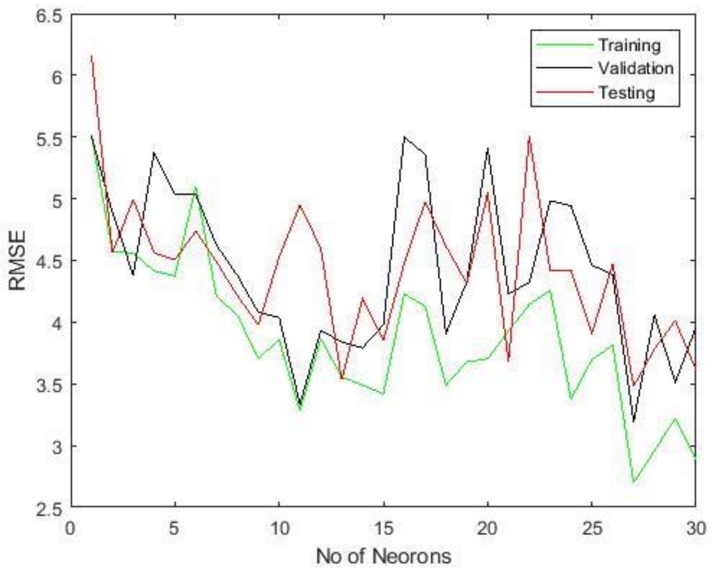

Fig. 7 Optimisation of the number of neurons adopted in the ANN for prediction of modulus of elasticity.

Based upon the optimisation process shown in Figure 7, the number of neurons adopted in the ANN is modified to 24, in order to minimise the RMSE. Subsequently, the linear regression for the observed predicted modulus of elasticity values were as follows (Fig. 8). Significant improvement in the performance can be observed after adjusting the numbers of neurons in the hidden layer from 10 to 24. The results are summarised in Table 3.

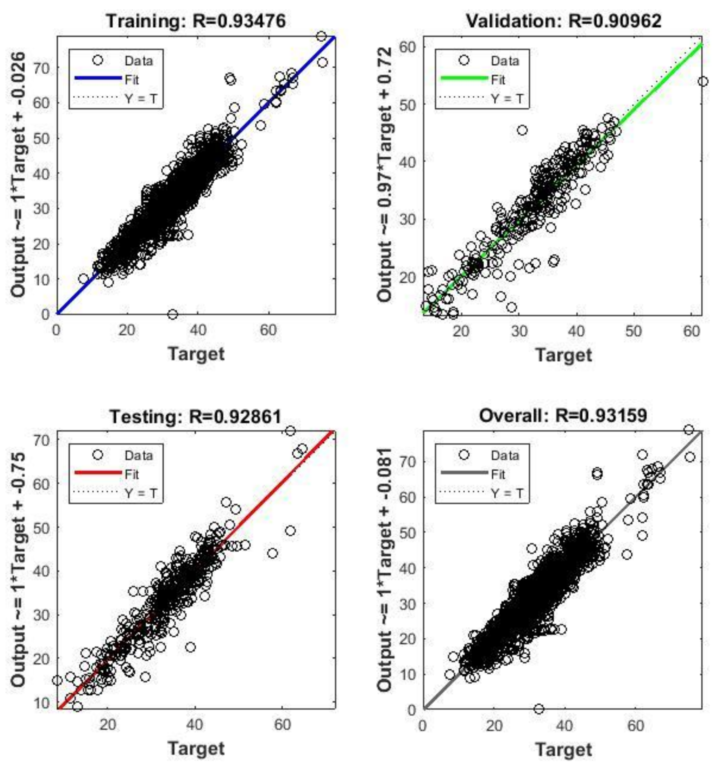

Fig. 8 Model performance: Predicted modulus of elasticity values of neural network compared with values actually observed in the laboratory for the testing examples using optimized number of neurons (24).

Table 3 Performance Comparison of RMSE for prediction Modulus of Elasticity

Performance Comparison in case of Compressive Strength		
State	RMSE (10)	RMSE Optimised (24)
Training	4.465	3.037
Validation	4.492	3.44
Testing	4.871	3.41

5.3 Tensile Strength:

Initially the model was trained with 10 number of neurons in the hidden layer, the performance of the model can be observed in the following regression plot (Fig. 9).

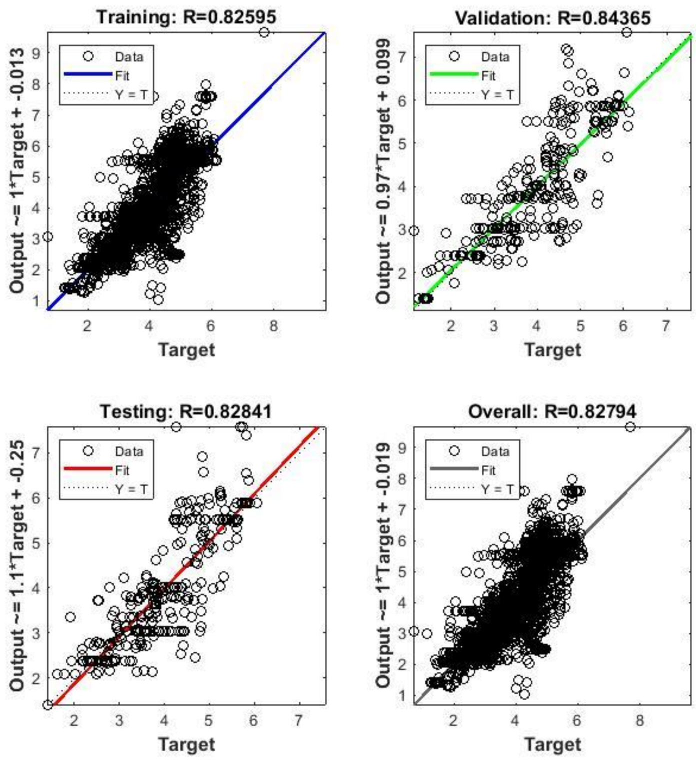

Fig. 9 Model performance: Predicted tensile strength values of neural network compared with values actually observed in the laboratory for the testing examples using number of neurons (10).

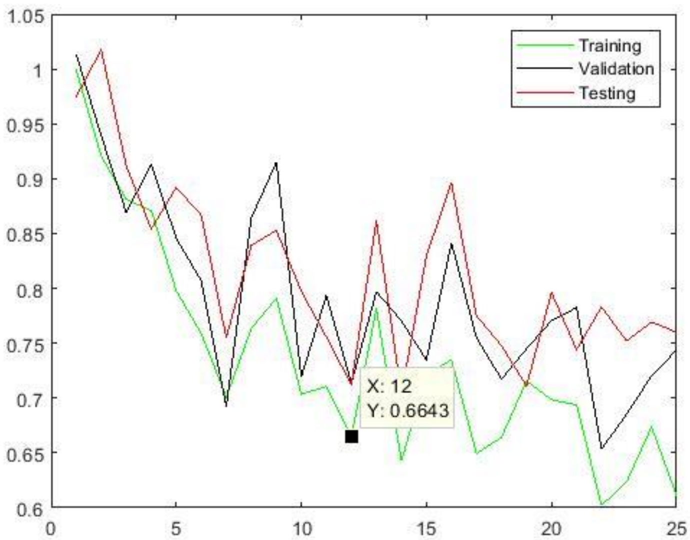

Fig. 10 Optimisation of the number of neurons adopted in the ANN for prediction of tensile strength.

The performance of the model in case of tensile strength is not good enough, exhibiting a sample correlation coefficient (R) close to 0.8. Therefore, as for the training of the ANN for compressive strength and modulus of elasticity training, the optimisation technique was adopted to calculate the optimum number of neurons. Results of the optimization process is shown as follows (Fig. 10).

Based upon the optimisation process shown in Figure 10, the number of neurons adopted in the ANN is modified to 15, in order to minimise the RMSE. Subsequently, the linear regression for the observed predicted modulus of elasticity values were as follows (Fig. 11).

6. Results

Upon validation of the ANN model, the model is utilised to evaluate the influence of different parameters, namely the percentage content of fly ash, Ground Granulated Blast Furnace Slag (GGBFS), and silica fume on the compressive strength, modulus of elasticity and tensile strength of Geopolymer concrete.

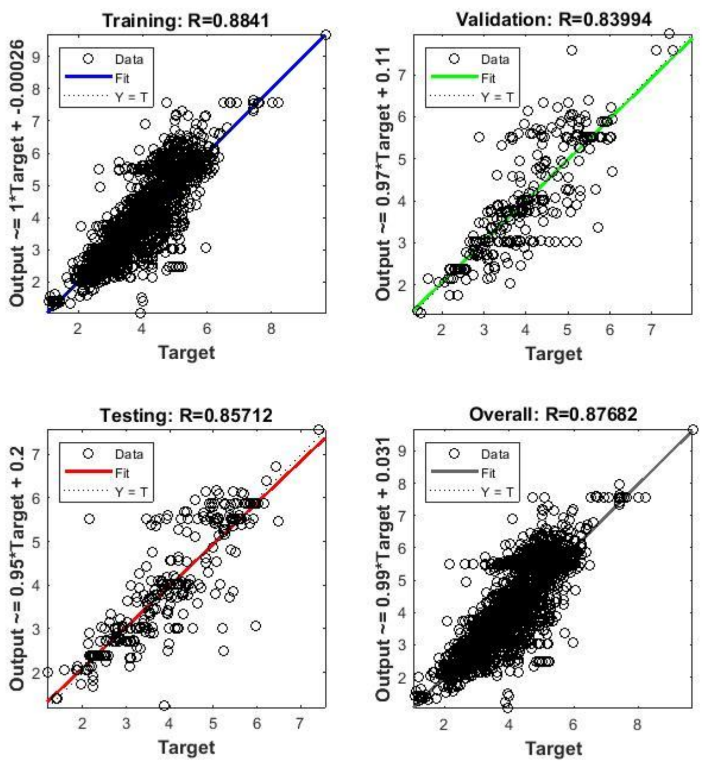

Fig. 11 Model performance: Predicted tensile strength values of neural network compared with values actually observed in the laboratory for the testing examples using optimized number of neurons (24).

Significant improvement in the performance can be observed after adjusting the numbers of neurons in the hidden layer from 10 to 24. The results are summarised in Table 4.

Table 4 Performance Comparison of RMSE for prediction Tensile Strength

Performance Comparison in case of Compressive Strength		
State	RMSE (10 neurons)	RMSE Optimised (15 neurons)
Training	0.750	0.62
Validation	0.735	0.732
Testing	0.732	0.717

Figure 12 presents the results of the predicted values for compressive strength by the ANN model, for admixture contents increasing in increments of 5% by mass.

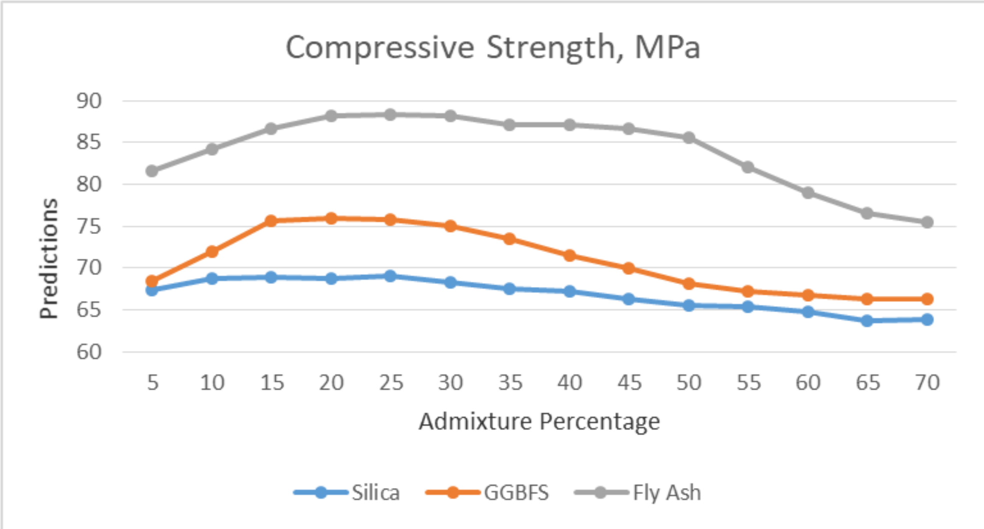

Fig. 12 Predicted compressive strength of concrete at 28 days

The results exhibited in Fig. 12 show that the compressive strength increases initially with increasing content of mineral admixtures, namely Silica Fume, Ground Granulated Blast Furnace Slag (GGBFS) and Fly Ash. However compressive strength is predicted to peak at percentage replacements ranging from 15-30% and begins to decrease beyond that. These results agree well with previous experimental studies (Bendapudi et al. 2011; Duval et al. 1998; Sharma et al. 2012).

Figure 13 presents the results of the predicted values for modulus of elasticity by the ANN model, for admixture contents increasing in increments of 5% by mass.

The results shown in Fig. 13 display a decrease in predicted modulus of elasticity of concrete with increasing fly ash content, which is agreeable with previous research (Atchley 1959; Mohammed Ali et al. 2020). For the remaining additives (Silica Fume and GGBFS), the results show minimal effect of increasing the percentage of additive by weight. The influence of these additives requires further research.

Figure 14 presents the results of the predicted values for tensile strength by the ANN model, for admixture contents increasing in increments of 5% by mass.

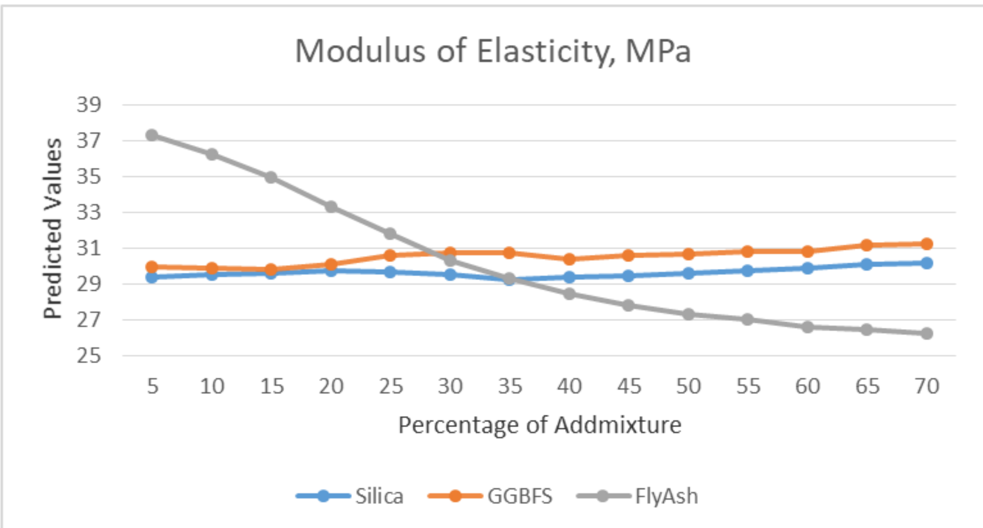

Fig. 13 Predicted Modulus of elasticity of concrete at 28 days .

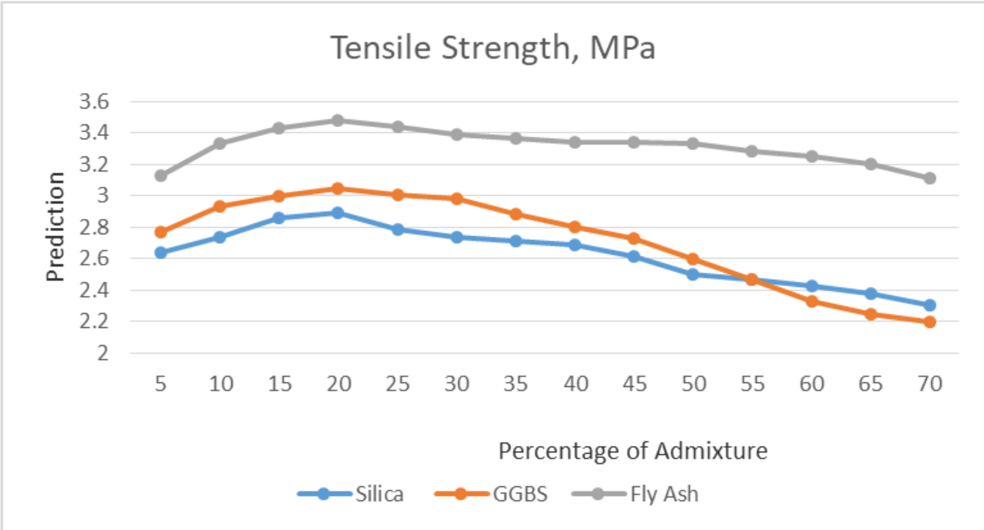

Fig. 14 Predicted Tensile Strength of concrete at 28 days.

The results shown in Fig. 14 show that the tensile strength increases initially with increasing content of mineral admixtures, namely Silica Fume, Ground Granulated Blast Furnace Slag (GGBFS) and fly ash. However, this trend only extends until about 15% replacement by mass, beyond which the tensile strength generally decreases as admixture content increases. These results are in good agreement with results of experimental procedures reported in the literature (Mohammed Ali et al. 2020; Smarzewski 2019).

7. Conclusions

Overall, the above results show that the ANN model is capable of predicting the mechanical properties of mineral additive enhanced high performance concretes. The results are generally in good agreement with previous experimental research. However, further research is required to enhance the accuracy of the model, and to predict mechanical properties with various percentages of multiple additives simultaneously. The results of this research may then be utilised to achieve higher utilisation of additives which would otherwise constitute hazardous waste materials in producing superior concretes for use in the construction industry, entailing both environmental and economic benefits.

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