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PREDICTION OF THE HIGH-TEMPERATURE PERFORMANCE OF A GEOPOLYMER MODIFIED ASPHALT BINDER USING ARTIFICIAL NEURAL NETWORKS

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ABSTRACT

Complexity in the behaviour of an asphalt binder is further escalated with geopolymer (fly ash and alkali liquid) modification, thus making it difficult to accurately predict the performance of the binder. This study employs artificial neural network modelling to predict the complex shear modulus, storage modulus, loss modulus and phase angle outcomes of experimental results from dynamic shear rheometer (DSR) oscillation tests under four separate scenarios. The proposed artificial neural network models received test conditions (temperature and frequency) and three different geopolymer concentrations (3%, 5% and 7% by the weight of bitumen) as the predictor parameters. The variants of the optimal algorithms were Levenberg-Marquardt (LM), Scaled conjugate gradient and Polak-Ribiere conjugate gradient (CPG) training algorithms with different combinations of network structures and tan-sig and log-sig as activation functions. The coefficient of determination, covariance and root mean square error (RMSE) were used as statistical measures of model prediction performance. Based on the statistical performance indicators, the LM algorithm with a 3-5-1 network architecture and tan-sig as the activation function was the best performing model for predicting the complex modulus with R^2 values of 0.996 for the training dataset and 0.971 for the testing dataset and RMSE values of 0.118 and 0.139 for the training and testing datasets, respectively. Furthermore, it was observed that the least efficient model was the phase angle prediction model developed with the CPG training algorithm, which had a 3-8-1 network architecture and log-sig as the activation function. The model yielded R^2 values of 0.909 and 0.829 for the training and testing datasets, respectively. Poor prediction performance for the testing dataset indicated that the model was unable to learn complexity in the data and would perform below a significance level of 0.90 in predicting using untrained data.

Keywords: Artificial neural networks; Complex shear modulus; Geopolymer modified asphalt binder; Loss modulus; Phase angle; Storage modulus

1. INTRODUCTION

Asphalt binder is a complex viscoelastic material that is predominantly used in highway construction (Ali et al., 2015; Ali et al., 2018). Asphalt binders are highly temperature susceptible, which means that they behave like elastic solids at cold temperatures and under low dynamic loading and behave like a Newtonian fluid at high temperatures and under heavy dynamic loading. The viscoelastic property of asphalt binders influences the high-temperature rutting and

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low-temperature thermal cracking failures of asphalt pavements (Tapkın et al., 2009). Asphalt pavements undergo repeated dynamic loading due to vehicular traffic (Du & Huang, 2012). A dynamic shear rheometer (DSR) was used in the experimental investigation of the rheological properties of binders at medium to high temperatures to simulate the dynamic loading effect and to evaluate the viscoelastic properties of asphalt binders, which significant for predicting the durability and service life of asphalt pavements (Al-Mansob et al., 2016). Complex modulus (G*) and phase angle (δ) are the two parameters revealed by the DSR oscillation test and are used to evaluate the viscoelastic behaviour of asphalt binders, as in the Superpave specification for the evaluation of asphalt cement for fatigue and rutting (Clyne et al., 2003). G* is the binder's resistance to deformation under repeated shear loading, and δ is the lag between the applied shear stress and the resulting shear strain. Larger δ values indicate more viscosity, while larger G* values are related to more elastic binders. The definition of δ and the relationship between the δ and G* are demonstrated in Figures 1 and 2. High elastic and low viscous properties are desired at low temperatures, whereas the high viscous and low elastic behaviour of asphalt binders are desired at high temperatures. On this basis, binder modification is a common practice and is referred to as modified asphalt cement (MAC).

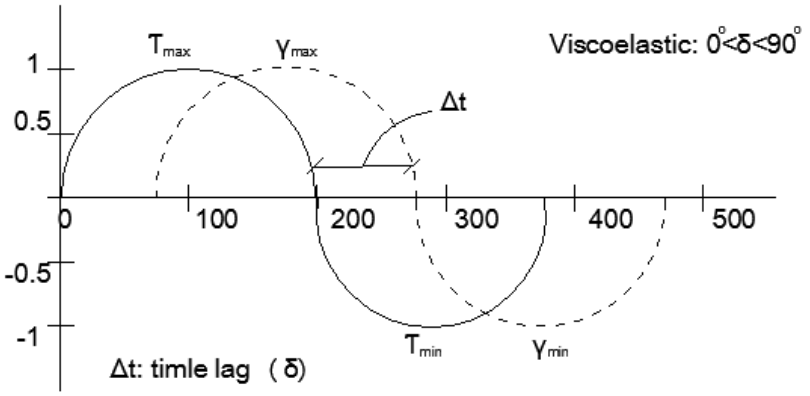

Figure 1 Definition of phase angle (Abedali, 2015)

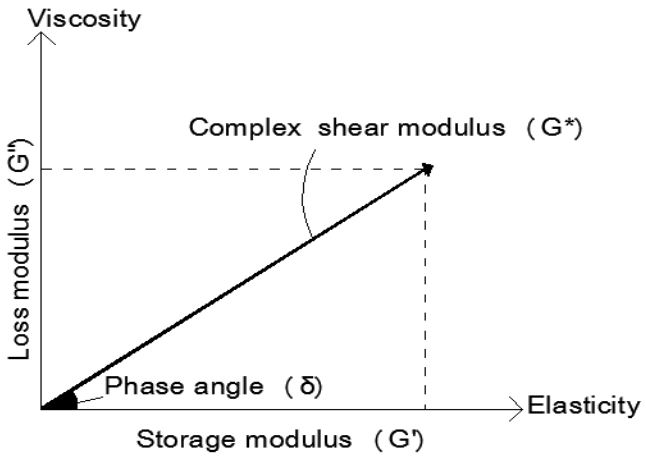

Figure 2 Viscoelastic behavior of bitumen (Abedali, 2015)

Bitumen modification with polymers and nanomaterials is a traditional and effective way to enhance the viscoelastic properties of asphalt binders. However, modification introduces further complexity to the behaviour of binders; hence, in order to determine optimum solutions, extensive

laboratory investigations are essential before field application (Fang et al., 2013). In recent years, some studies have presented mathematical and computational methods to model the behaviour of modified asphalt binders to eliminate or provide assistance for the experimental procedures. Some of the successful modelling techniques include numerical modelling using finite element analysis, mathematical modelling using regression models, statistical modelling using response surface methodology (RSM) and heuristic prediction techniques (Huang et al., 2015; Venudharan & Biligiri, 2017; Ziari et al., 2018). Artificial neural networks (ANN) are heuristic prediction techniques that have been gaining the attention of researchers in the field of material science as acknowledged in the literature (Tasdemir, 2009). Baldo et al. (2018) utilized the ANN modelling technique to analyse the mechanical behaviour of asphalt concretes using base bitumen and polymer modified bitumen data observed through experimental investigations. The models developed in their study included single outputs of four mechanical parameters, namely Marshall stability, flow, quotient and stiffness modulus and input parameters, including the bitumen type, the bitumen content, the filler-bitumen ratio, air voids, voids in the mineral aggregates, voids filled with bitumen and the type of production process. Their study produced satisfactory results of correlation coefficient values in the range of 0.98798–0.91024 with the testing dataset. Furthermore, closed-form equations for all four models were developed for repeatability of the results with different materials within the framework provided in their study. The feasibility of the application of ANN in pavement engineering is discussed in Section 2. ANN is a modelling technique used for the classification, regression and prediction of non-linear datasets by learning from supplementary data and predicting new data based on the learned pattern of the data (Zuna et al., 2016; DeRousseau et al., 2018). ANN consists of three layers, including the input layer, in which the predictor variables are fed to the network; the hidden layer, which is the middle layer; and the output layer, in which the network targeted variables are predicted. The performance of ANN strongly depends on the type of data as well as dataset congruence with network features such as the network topology, the training algorithm and the activation function. Readers are referred to (Baldo et al., 2018) for a detailed description of the mathematical theory behind the modelling of neural networks.

The objective of this study was to evaluate the prediction performance of ANN models developed under four separate scenarios with different combinations of ANN architectures, training algorithms and activation functions to predict complex shear modulus (G*), phase angle (δ), storage modulus (G') and loss modulus (G'') by using test conditions (temperature and frequency) and different geopolymer concentrations (3%, 5% and 7% by the weight of binder) in order to eliminate the drawbacks of the experimental procedures.

2. LITERATURE ARTIFICIAL NEURAL NETWORKS OVERVIEW

Laboratory investigation of asphalt materials can be time and resource intensive. Therefore, many researchers have attempted to develop statistical and computational models to predict the performance characteristics of asphalt materials in order to replace physical experimentation or to gain insight into the probable outcomes of experiments (Sebaaly et al., 2018). ANN is a soft computing technique which operates by learning from assistive data provided to the network to analyse the patterns in the data and to predict new data based on learned data (Naderpour & Mirrashid, 2018). The feasibility of the application of ANN models in the area of asphalt pavement performance has only been explored in a limited number of research studies. Furthermore, these attempts were mainly focused on concrete mixtures and asphalt mixtures, while very few studies have attempted to use ANN to model the performance characteristics of asphalt binders, which have a significant influence on the overall performance and lifespan of asphalt pavements (Kok et al., 2010). In a study conducted by (Tapkın et al., 2009), the prediction of strain accumulation for polypropylene modified Marshall Specimens in a repeated

creep test was modelled using artificial neural networks. The results of their study showed that the neural network model provided a high prediction capacity of the actual performance characteristics and that it could be used as a replacement for destructive experimental procedures. Liu et al. (2018) studied the potential application of neural networks and Iowa models to predict the dynamic modulus of asphalt mixtures containing recycled asphalt shingles. Through sensitivity analysis, it was found that neural network models outperformed the Iowa models. El-Badawy et al. (2018) compared regression models and ANN models with Witczak NCHRP 1-37A, Witczak NCHRP 1-40D and Hirsch E* predictive models for predicting the dynamic modulus of hot mix asphalt. The database contained the test results of volumetric properties, aggregate gradations, binder viscosity, complex shear modulus and phase angle experimental results obtained from different mixes. The ANN models using the same input parameters yielded better performance for the three predictive models than the regression models. According to Firouzinia and Shafabakhsh (2018), asphalt pavements are highly temperature susceptible and in addition to binder modification, asphalt mixture should also be modified to overcome this problem. Five different silica modifier concentrations were used in their study, and, along with the experimental investigation, neural network models were developed. The temperature sensitivity of asphalt mixture was improved, and ANN models were able to predict the experimental results sufficiently.

In recent years, there have been several studies dedicated to computational modelling of asphalt binders. Venudharan and Biligiri (2017) used heuristic principles to predict the rutting performance of crumbed rubber modified binders. In their study, the effects of five different crumbed rubber gradations were investigated. Eight different input parameters, including physical properties of the modified binder, mechanical test conditions and different rubber gradations, were used to predict the rutting performance. The various combinations of neural network architectures with different algorithms of training and transfer functions were trained, and a backpropagation learning algorithm with scaled conjugate function (SCG) as the training algorithm in a feedforward, two-hidden layer neural network with seven and three neurons was found to be the optimum model. The styrene-butadiene-styrene (SBS) modified asphalt binder was modelled using artificial neural networks in a study conducted by (Kok et al., 2010). Temperature and frequency conditions along with different SBS concentrations were used as inputs to predict the complex modulus of the asphalt binder. The study adopted various combinations of ANN architectures and learning algorithms, such as Levenberg-Marquardt (LM), Scaled Conjugate Gradient and Pola-Ribiere Conjugate Gradient, and it was revealed that the LM algorithm was the most optimal topology for predicting the complex modulus. Abedali (2015) conducted a study that compared the performance of Multiple Linear Regression (MLR) models and ANN with a base asphalt binder. The input parameters included temperature, frequency, dynamic viscosity, shear stress and strain, and the output parameter was the complex modulus. Ziari et al. (2018) conducted a similar comparison study using carbon nanotube (CNT) modified asphalt binders to predict the rutting performance. In both studies, ANN models were acknowledged to perform significantly better than the MLR models.

3. MATERIALS AND METHODS

3.1. Materials and Experimental Methods

The 60/70 penetration grade was used as the base asphalt, and a combination of fly ash and alkali liquid was the geopolymer used as a modifier of asphalt binders. The alkali liquid was a sodium silicate solution (Na_2SiO_3) and sodium hydroxide (NaOH) pallet diluted in water to produce an 8 Molar (8M) NaOH solution, while the fly ash class F had a specific gravity of 2.26. A combination of Na_2SiO_3 and NaOH was prepared to activate the alumino-silicate precursors in fly ash through a series of dissolution-hydrolysis (Ali et al., 2017). The data used in ANN

modelling was obtained from physical tests (penetration, softening point, viscosity), which were conducted according to ASTM D5, ASTM D36 and a rheological test using a dynamic shear rheometer (Frequency sweeps tests), which was conducted according to AASHTO T315.

3.2. Artificial Neural Networks Modelling

An ANN is a machine learning system designed to model nonlinear classification, regression and prediction problems involving high complexity (DeRousseau et al., 2018). ANNs are inspired by the way biological neurons work in the human brain. They consist of highly interconnected artificial neurons, which adopt a multi-layered perceptron (MLP) structure, as shown in Figure 3, to model complex nonlinear problems, for which standard mathematical models are inadequate (Esen et al., 2008; Chandwani et al., 2015).

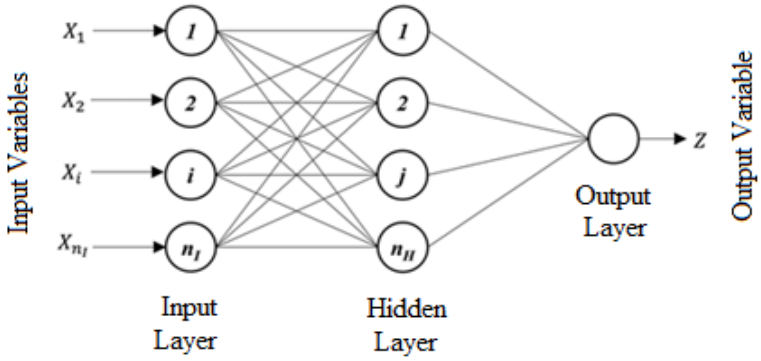

Figure 3 Overview of feed forward MLP model

The models developed herein consisted of three layers: an input layer, a hidden layer, and an output layer. The range of the dataset for these layers was based on experimental observations. Prior to modelling, the data were pre-processed by the Z-score normalization technique to reduce the effect of variance and to ensure that the data was in the compatible range (Ziari et al., 2018).

3.3. Artificial Neural Networks Data Analysis

Matlab (MathWork Inc R2013a) was used to develop ANN models for the data observed from the DSR oscillation tests. Four separate models were developed using mechanical test parameters (Temperature [T] and Frequency [f]) and three different polymer concentrations (PC) namely (3%, 5% and 7% by the weight of binder) as input parameters in order to predict different outputs in four separate scenarios, which were complex modulus (G*), phase angle (δ), storage modulus (G') and loss modulus (G''), as explained in Equations 2–5. Before developing neural network models, the data was pre-processed using the z-score normalization expressed in Equation 1 to reduce data redundancy and improve data integrity.

$$z = \frac{(x-\mu)}{\sigma} \tag{1}$$

where z is the normalized score, x is the observed data, μ is the arithmetic mean, and σ is the standard deviation.

Scenario 1: $x_1 = Normalized\{T, f, PC\}$ $y_1 = Normalized\{G^*\}$ (2)

Scenario 2: $x_2 = Normalized\{T, f, PC\}$ $y_1 = Normalized\{\delta\}$ (3)

Scenario 3: $x_3 = Normalized\{T, f, PC\}$ $y_1 = Normalized\{G'\}$ (4)

Scenario 4: $x_4 = Normalized\{T, f, PC\}$ $y_1 = Normalized\{G''\}$ (5)

A feedforward neural network (FFNN) with the backpropagation method was used. The multi-layered perceptron (MLP) was constructed using various learning algorithms, different transfer functions and a hidden number of neurons. The optimum models were found using various combinations of the abovementioned ANN architectures in Section 3.2 by trial and error. The approach to modelling was supervised learning. A total of 252 sets of data were randomly divided into two groups, where 70% of the experimentally observed data were used for training the model, and 30% of the data were used for testing the model for unlearned data. During the training phase, initial weights were randomly generated and through an iterative process were rearranged to find the most accurate predictions of the actual data. However, this can cause the network to fall into a local minimum, or the issue of overfitting may occur. Therefore, the optimum model selection was performed through an iterative process by finding the optimum epoch number, which is a measure of the number of times all the training vectors are used once to update the weights (Huang et al., 2015). Models developed for training and testing datasets were analysed for their model prediction capacity. The optimum network structures were evaluated by performance indicator metrics, which were RMSE, Coefficient of determination (R^2) and Covariance (COV), as given by Equations 6–8.

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(\hat{\gamma}_i - \gamma_i)^2} \tag{6}$$

$$R^2 = 1 - \left[\frac{(\gamma-\hat{\gamma})^2}{(\gamma-\gamma_{mean})^2}\right] \tag{7}$$

$$COV = \left[\frac{RMSE}{|\widehat{\gamma_{mean}}|} \times 100\right] \tag{8}$$

where $\hat{\gamma_i}$ is a vector denoting the values of n number of target values, and γ_i is a vector representing experimentally observed values.

4. RESULTS AND DISCUSSION

The prediction capacity of the constructed networks was strongly influenced by the nature of the dataset (Liu et al., 2018). In this vein, various network topologies with different learning algorithms and activation functions explained in Section 3.3 were attempted before finding the optimum networks for each model. Four separate models, which were expected to predict experimentally observed values for complex modulus, phase angle, storage modulus and loss modulus, were constructed. Among the learning algorithms, LM for predicting complex modulus and storage modulus, Polak-Ribiere conjugate gradient (CPG) for predicting phase angle and SCG for predicting the loss modulus were found to be the most suitable algorithms for the developed models.

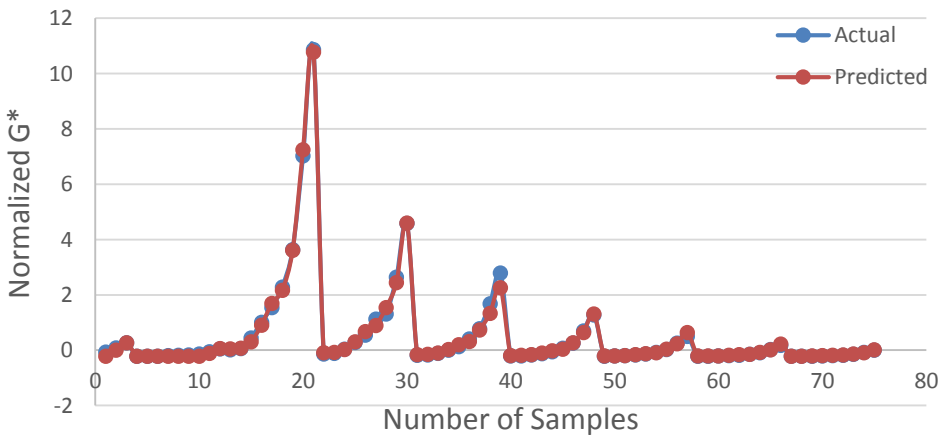

Figure 4a Comparison between actual and ANN predicted for G*

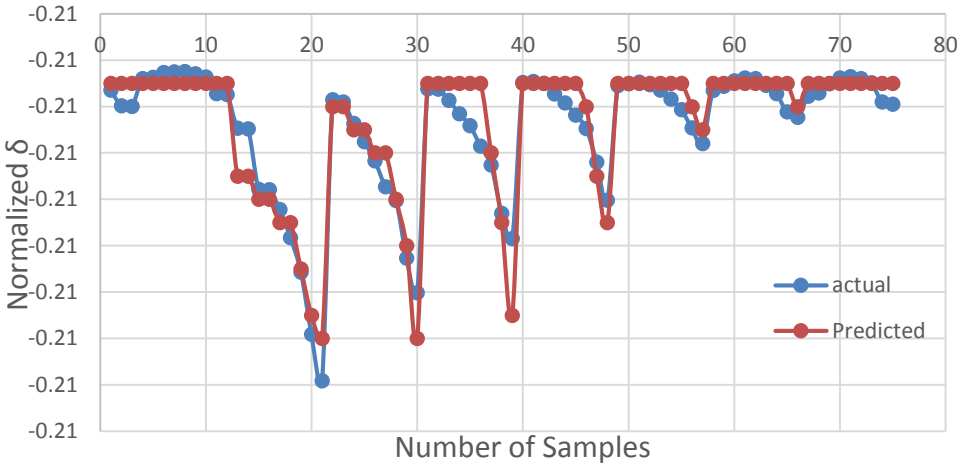

Figure 4b Comparison between actual and ANN predicted for δ

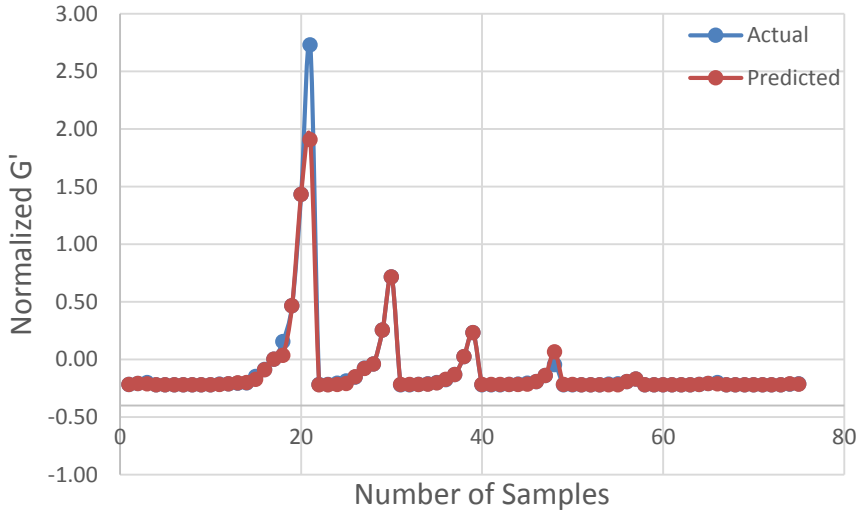

Figure 4c Comparison between actual and ANN predicted for G’

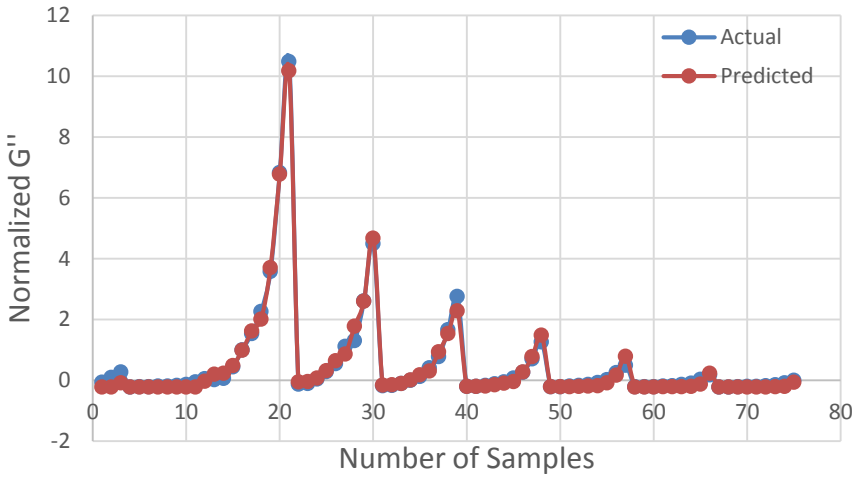

Figure 4d Comparison between actual and ANN predicted for G”

The network structure for the phase angle predictive model was constructed as three input neurons, a hidden layer with eight neurons and one output neuron, and a log-sigmoid function was adopted as the activation function. The remaining networks were constructed as three input neurons, a hidden layer with five neurons and one output neuron, and the tan-sigmoid activation function was adopted in order produce optimal prediction capacity models. The R^2 value was used as a statistical measure of the prediction performance of the models. R^2 values close to 1 indicated that the model had a high accuracy at predicting the target dataset, whereas values below 0.9 were considered insensitive at learning the pattern in the data; they also indicated that the model prediction capacity was not sufficient. In Figures 4a–4d, a point-to-point comparison was further demonstrated between the actual experimental data and the model predicted data for all models. As illustrated in Figure 5, R^2 values higher than 0.9 were observed with both training and testing datasets in the three scenarios which were modelled for predicting G*, G' and G''. On the other hand, the lowest prediction capacity was observed with the model developed for δ prediction.

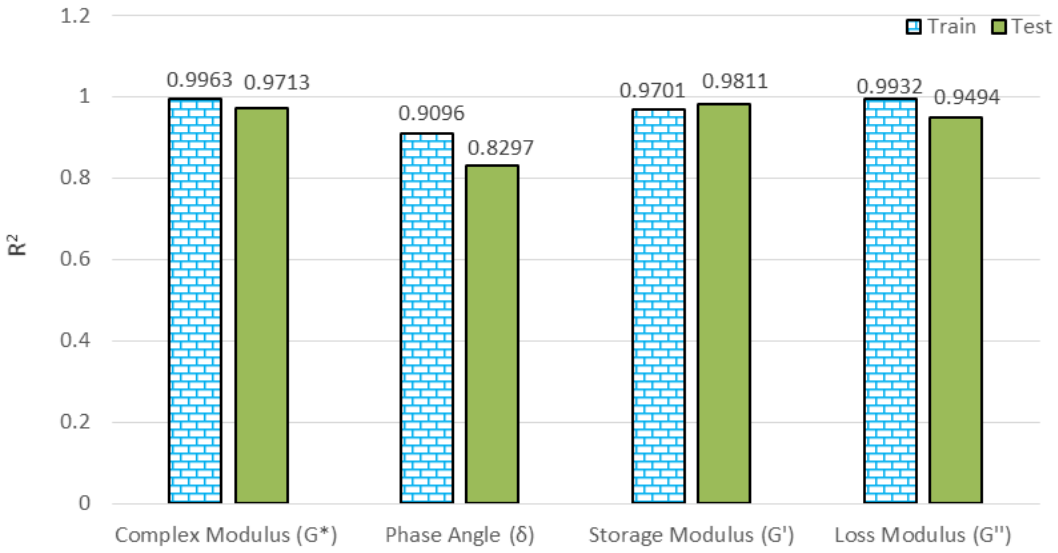

Figure 5 R^2 values for training algorithms

Among the four models, the most precise model was achieved with the G* prediction model developed with the LM training algorithm, a hidden layer with five neurons and tan-sig as the activation function. R^2 values of 0.996 and 0.971 were found for the training and testing datasets, respectively. Following that, the G'' prediction model was perceived as the second optimal model, where R^2 values of 0.993 with the training dataset and 0.949 with the testing dataset were obtained with the tan-sig activation function and a network topology of 3-5-1. For the storage modulus prediction model, R^2 values of 0.970 for the training and 0.891 for the testing datasets were observed. Although the network performed satisfactorily with the training dataset, the lower R^2 value for the testing dataset indicated that the model prediction performance would not be as precise for the untrained datasets. Furthermore, it was observed that the model developed with the CGP training algorithm, which adopted log-sigmoid as activation and had a network structure of 3-8-1, poorly captured the complex non-linear relationship of data, producing R^2 values of 0.909 and 0.830 for the training and testing datasets, respectively. Other statistical parameters used for the model performance evaluation, including RMSE and covariance criteria, are given in Table 1.

Table 1 Statistical model performance indicators

Variable Name	Model Type	R^2	RMSE	COV
Complex Modulus (G*)	Training dataset	0.996393	0.117599	22.41395
	Testing dataset	0.971301	0.138542	29.96316
Phase Angle (δ)	Training dataset	0.909607	0.00014	0.066091
	Testing dataset	0.829744	0.000554	0.26105
Storage Modulus (G')	Training dataset	0.970131	0.105886	98.90051
	Testing dataset	0.891086	0.38146	268.197
Loss Modulus (G'')	Training dataset	0.993214	0.000863	156.6776
	Testing dataset	0.949393	0.204787	40.78695

5. CONCLUSION

The objective of this study was to develop and evaluate the performance capacity of ANN models to predict experimental results from DSR oscillation tests. G*, δ, G' and G'' were attempted to be predicted from mechanical test conditions for modified asphalt binders with the addition of 3%, 5% and 7% geopolymer composed of fly ash and alkali liquid.

The following conclusions can be drawn from this study: (1) The best performing model was developed for predicting G*. The features of the model included an LM training algorithm, tan-sig activation function and 1-5-1 network structure. The model performance evaluated by R^2, RMSE and COV produced metrics of 0.996, 0.117 and 22.41, respectively; (2) Models developed for predicting G' and G'' performed satisfactorily regarding performance indicator metrics. However, the variation observed in the R^2 values between the training and testing data was an indication that the performance of the models may not have been as precise for predicting untrained datasets; (3) Based on the R^2 results, the model developed for predicting δ was observed as the least efficient model regarding prediction capacity.

The value of 0.823 with the testing dataset revealed that the model was unable to learn complexity in the data and that it would perform poorly with untrained new datasets.

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