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

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Abstract- Complexity in the behavior of asphalt binders are further escalated with geopolymer (fly ash and the alkali liquid) modification thus, making it difficult to predict the performance of the binder accurately. This study employs artificial neural network modelling in order to predict complex shear modulus, storage modulus, loss modulus and phase angle outcomes of experimental results from 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%.wt by the weight of bitumen) as the predictor parameters. The variants of the optimal algorithms were Levenberg-Marquardt, Scaled conjugate gradient and Polak-Ribiere conjugate gradient 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 squared error were used as statistical measures of model prediction performance. Based on the statistical performance indicators Levenberg-Marquardt algorithm with 3-5-1 network architecture and tan-sig as activation function was the best performing model for predicting complex modulus with R^2 values of 0.996 for training dataset and 0.971 for testing dataset and RMSE values of 0.118 and 0.139 for training and testing datasets respectively. Further, it was observed that the least efficient model was phase angle prediction model developed with the Polak-Ribiere conjugate gradient training algorithm, 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 training and testing datasets respectively. Poor prediction performance for the testing dataset was an indication that the model was unable to learn complexity in the data and that would perform below 0.90 significance level at predicting with untrained data.

Keywords- Geopolymer modified asphalt binder; artificial neural networks; complex shear modulus; storage modulus; loss modulus; phase angle

1. INTRODUCTION

Asphalt binders are highly temperature susceptible, which behaves like an elastic solid at cold temperatures and under low dynamic loading and behaves like a Newtonian fluid at high temperatures and under heavy dynamic loading. Viscoelastic property of asphalt binders influences the high-temperature rutting and low temperature thermal cracking failures of asphalt pavements (Tapkın et al., 2009)

Asphalt pavements are under repeated dynamic loading due to vehicular traffic. A dynamic shear rheometer (DSR) is used in the experimental investigation of rheological properties of binders at medium to high temperatures in order to simulate the dynamic loading effect and to evaluate the viscoelastic properties of asphalt binders which is of significance at predicting the durability and service life of asphalt pavements (Venudharan and Biligiri, 2017). Complex modulus (G*) and phase angle (δ) are the two parameters revealed by DSR oscillation test which are used to evaluate the viscoelastic behavior of asphalt binders as used in the Superpave specification for grading of asphalt cement for fatigue and rutting (Abedali, 2015). G* is the binders 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 relate to the more viscous binder, while larger G* values are related to more elastic binder (Interactive, 2016). 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, and high viscous and low elastic behavior of asphalt binders are desired at high temperatures. On this basis, binder modification is a common practice and referred to as modified asphalt cement (MAC) (Abedali, 2015).

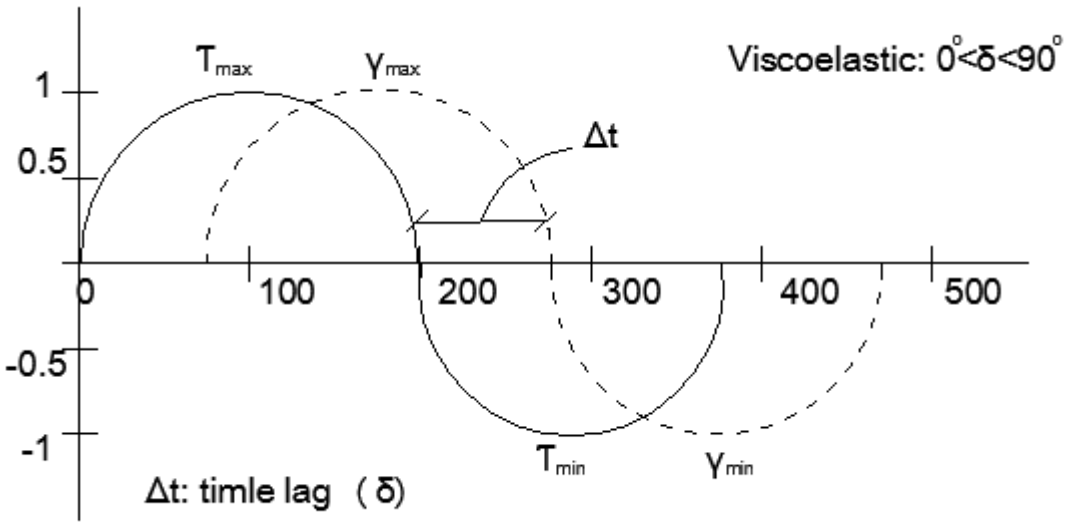


Figure 1: Definition of phase angle (Abedali, 2015)

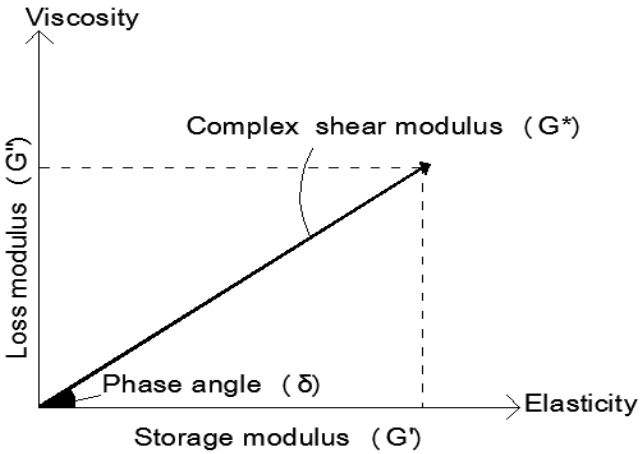


Figure 2: Viscoelastic behavior of bitumen (Abedali, 2015)

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 in the behavior of binders and hence, to find optimum solutions, extensive laboratory investigations are essential before field application (Fang et al., 2013). In recent years, some studies presented mathematical and computational methods to model the behavior of modified asphalt binders to eliminate or providing assistance for the experimental procedures. Some of the successful modeling techniques include numerical modeling using finite element analysis, mathematical modeling using regression models, statistical modeling using response surface methodology (RSM) and heuristic prediction techniques (Ziari et al., 2018, Venudharan and Biligiri, 2017, Huang et al., 2015).

Artificial neural networks (ANN) is among the heuristic prediction techniques which has been gaining the attention of researchers in the field of material science as acknowledged in the literature (Golzar et al., 2012, Specht et al., 2007, Tasdemir, 2009). Aformentioned literature and as detailed in the artificial neural networks overview section, have proven the tangibility of application of ANN in pavement engineering. ANN is a modeling technique used for 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 (DeRousseau et al., 2018). ANN consists of three layers namely input layer which the predictor variables are fed to the network, hidden layer which is the middle layer and output layer which the network targeted variables are predicted. The performance of ANN strongly depends on the type of data, and dataset congruence with network features such as the network topology, the training algorithm and activation function used. The objective of this study was to evaluate the prediction performance of ANN models developed under 4 separate scenarios with different combinations of ANN architectures, training algorithms and activation functions to predicting 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) to eliminating the drawbacks of experimental procedures.

2. ARTIFICIAL NEURAL NETWORKS OVERVIEWS

Laboratory investigation of asphalt materials is time and resource intensive. Therefore, many researchers have attempted to develop statistical and computational models to predicting performance characteristics of asphalt materials to replace physical experimentation or to have a primary insight about the probable outcomes of the experiments (Sebaaly et al., 2018). ANN is among the soft computing techniques which operate by learning from assistive data provided into the network to analyzing the pattern in the data and predicting new data based on learned data (Naderpour and Mirrashid, 2018). The tangibility of application of ANN models in the field of performance of asphalt pavements was explored in limited research studies. However, these attempts were mainly focused on concrete mixtures, and asphalt mixtures and very few studies have attempted to use ANN for modeling the performance characteristics of asphalt binders, which are strong influencers of the overall performance and lifespan of asphalt pavements (Kok et al., 2010).

In a study conducted by (Tapkın et al., 2009), prediction of strain accumulation for polypropylene modified Marshall specimens in repeated creep test was modeled using artificial neural networks. The results of their study showed that the neural network model provided high prediction capacity of the actual performance characteristics and that it could be used in replacement for destructive experimental procedures. (Liu et al., 2018) Studied the potential application of neural networks and Iowa models to predicting 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 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 three predictive models than 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. Temperature sensitivity of asphalt mixture was improved, and ANN models were able to predict the experimental results sufficiently.

In recent years there have also been several studies dedicated to computational modeling of asphalt binders. (Venudharan and Biligiri, 2017) Used heuristic principles for predicting the rutting performance of crumbed rubber modified binders. In their study, the effect of 5 different crumbed rubber gradations was 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 backpropagation learning algorithm with SCG as the training algorithm in a feed forward, two hidden layers neural network with seven and three neurons were found to be the optimum model. SBS modified asphalt binder was modeled 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 for predicting complex modulus of the asphalt binder. The study adopted various combinations of ANN architectures and learning algorithms such as Levenberg-Marquardt, Scaled Conjugate Gradient, and Pola-Ribiere Conjugate Gradient, and it

was revealed that Levenberg-Marquardt algorithm was the most optimal topology for predicting complex modulus. (Abedali, 2015) Conducted a comparison study between the performance of Multiple Linear Regression models (MLR) and ANN with base asphalt binder. Input parameters included were temperature, frequency, dynamic viscosity, shear stress, and strain and the output parameter was complex modulus. A similar comparison study was conducted with carbon nanotube (CNT) modified asphalt binders to predicting the rutting performance by (Ziari et al., 2018). In both studies, ANN models were acknowledged to perform significantly better than the MLR models.

2. EXPREMTEAL DATA ACQUISITION

2.1. Materials Experimental Methods

The 60/70 penetration grade was used as the base asphalt, and the combination of fly ash and the alkali liquid was geopolymer used as a modifier of asphalt binders. The alkali liquid was sodium silicate solution (Na_2SiO_3) and sodium hydroxide (NaOH) pallet diluted in water to produce 8 Molar (8M) NaOH solution, while The fly ash class F with 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. The data used in ANN modeling was obtained from physical tests (penetration, softening point, viscosity) which conducted according to ASTM D5, ASTM D36, and rheological test using dynamic shear rheometer (Frequency sweeps tests) which conducted according to with AASHTO T315.

2.2. Artificial Neural Networks Modeling

ANN is a machine learning system designed to model nonlinear classification, regression and prediction problems involving high complexity (DeRousseau et al., 2018). ANN is inspired by the way biological neurons work in the human brain. It consists of highly interconnected artificial neurons, which adopts multi-layered perceptron (MLP) structure as shown in Figure 3 to model complex nonlinear problems that standard mathematical models are inadequate (Abdullah, 2009).

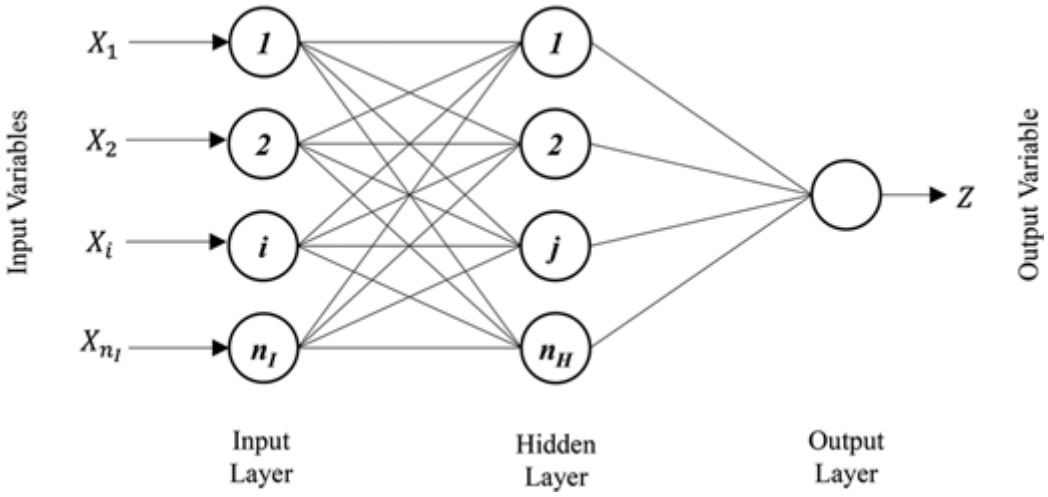


Figure 3: Overview of Feed Forward MLP model

Models developed herein consisted of three layers namely, an input layer, hidden layer, and an output layer. Based on experimental observations, the range of data set for these layers can be seen in Table 1. Before modeling, the data were preprocessed by Z-score normalization technique to reduce the effect of variance and also that, the data was in the compatible range (Ziari et al., 2018).

Table 1: Input and output parameters

Variable Type	Variable name	Experimental Data Range	Normalized Data Range
Input Parameters	Polymer Concantration (%)	0-7	(-0.21991) - (-0.21929)
	Temperature (C)	46-82	(-0.21576) - (-0.21251)
	Frequency (Hz)	0.159-15.92	(-0.21990) -(-0.21848)
Output Parameters	Complex modulus (Pa)	10.86-8616	(-0.21893) - 17.14353
	Phase angle (^{o})	78.75-88.72	(-0.21614) - (-0.21184)
	Storage modulus (Pa)	0.791-1680	(-0.21987) - 4.872578
	Loss modulus (Pa)	10.83-8450	(-0.21894) - 16.37564

The type of network used in this study was feed forward neural network with back propagation method. In this type of networks, the input layer feeds the data for the input parameters and output layer produces predictions for the experimentally observed output data. Initial weights were randomly assigned and by performing forward and backward calculations, developed models, attempted to find the closest predictions to actual dataset fed to the network (Jung and Ghaboussi, 2006). The model prediction capacity was influenced by several factors such as the learning algorithm, activation function and some hidden neurons used in the network (Abdullah, 2009). Matlab has some learning algorithms such as Levenberg Marquardt, Gradient Descent, Scaled Conjugate Gradient, etc. and activation functions such as sigmoidal, hard limiter and hyperbolic tangent functions to perform training with backpropagation method (Ziari et al., 2018). Therefore, finding the optimum network model is an iterative, trial and error process and it was as approached in this study. To determine the optimum model, common statistical metrics approached in the literature include, Mean Absolute Error (MAE), Mean Squared Error (MSE), Root Mean Squared Error (RMSE), Average Percentage Error (APE) and Coefficient of Determination (R^2) (Ziari et al., 2018, Dutta et al., 2017, Kok et al., 2010). In this study, RMSE, Covariance (COV) and R^2 were adopted for evaluating the prediction capacity of the models developed.

2.3. Artificial neural networks data analysis

Matlab (MathWork Inc R2013a) was used to develop ANN models for the data observed from the DSR oscillation tests. 4 separate models were developed using mechanical test parameters (Temperature (T) and Frequency (f)) and 3 different polymer concentrations (PC) namely (3%, %5 and 7% by the weight of binder) as input parameters in order to predicting different outputs in 4 separate scenarios which were complex modulus (G*), phase angle (δ), storage modulus (G') and loss modulus (G'') as explained in eqn.2-5. Before developing neural network models, the data was preprocessed using z-score normalization expressed in eqn. 1 to reduce data redundancy and improving data integrity (Mohabeer et al., 2011).

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

Where; z: Normalized score, x: Observed data, μ: Arithmetic mean and σ: 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)

The type of network used was fed forward neural network (FFNN) with backpropagation method. Multi-layered perceptron (MLP) were constructed using various learning algorithms, different transfer functions and hidden number of neurons. The optimum models were found using various combinations of abovementioned ANN architectures in the Artificial Neural Networks Modelling section by trial and error. The approach to modeling was supervised learning. 252 set 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, rearranged for finding the most accurate predictions of the actual data. However, this may 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. An epoch is a measure of the number of times all the training vectors are used once to update the weights (Venudharan and Biligiri, 2017).

Models developed for training and testing datasets were analyzed for model prediction capacity. The optimum network structures were evaluated by performance indicator metrics which were Root Mean Squared Error (RMSE) and Coefficient of determination (R^2) and Covariance (COV) as given by eqn. 6- eqn. 8

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

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

$$COV = \left[\frac{RMSE}{|\hat{\gamma}_{mean}|} \times 100\right] \quad (8)$$

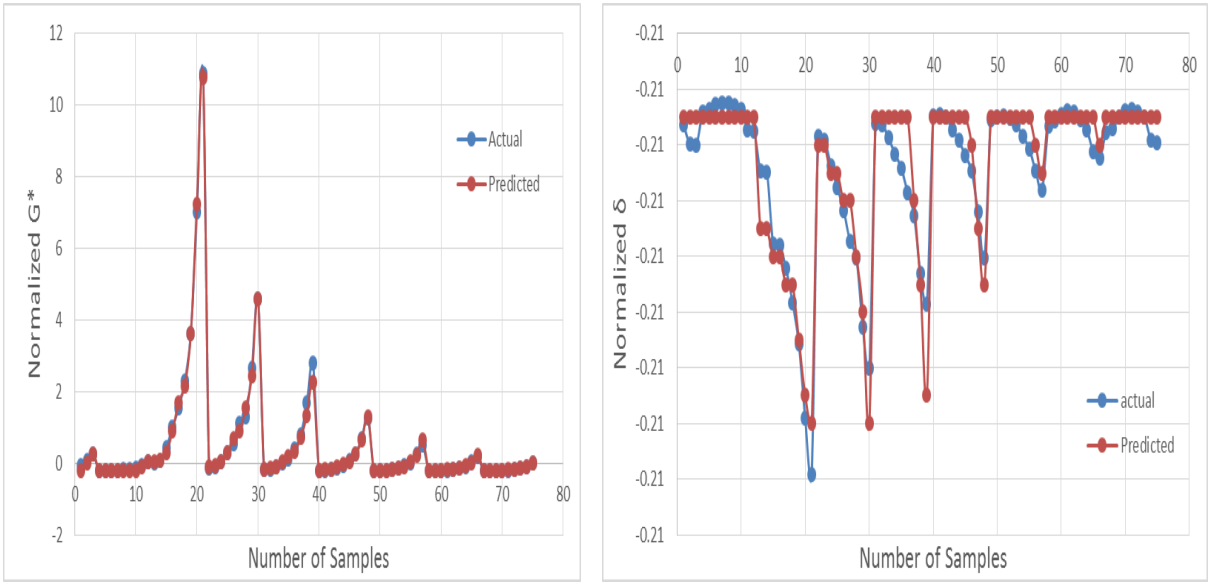
Where; γˆ_i is vector denoting values of n number of target values, γ_i is a vector representing experimentally observed values.

3. RESULTS AND DISCUSSION

3.1. Artificial Neural Networks Model Results

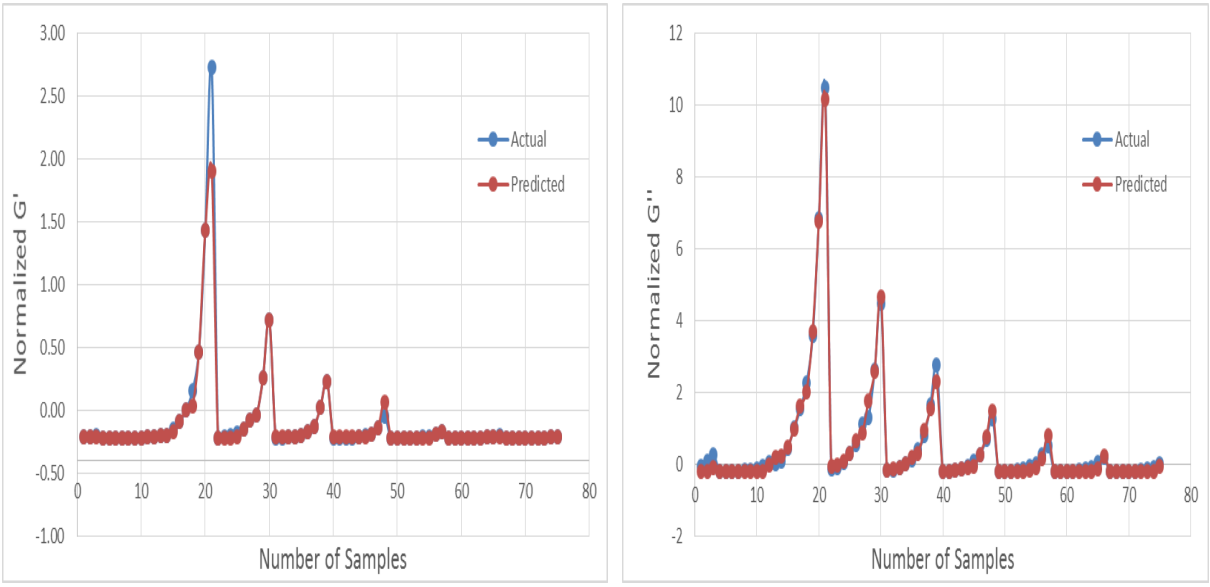
The prediction capacity of the networks constructed was strongly influenced by the nature of the dataset. In this vein, various network topologies with different learning algorithms and activation functions explained in the artificial neural network data analysis section were approached before finding the optimum networks for each model. Four separate models were constructed which were expected to predict experimentally observed values for complex modulus, phase angle, storage modulus, and loss modulus. Among the learning algorithms Levenberg-Marquardt (LM) for predicting complex modulus and storage modulus, Polak-Ribiere conjugate gradient (CPG) for predicting phase angle and scaled conjugate function (SCG) for predicting the loss modulus were found to be the most suitable algorithms for the developed models. The network structure for phase angle predictive model was constructed as three input neurons, 8 number of hidden neurons and one output neuron and adopted log-sigmoid function as the activation function. The remaining networks were constructed as three input neurons 5 number of hidden neurons and one output neuron and adopted tan-sigmoid activation function as to produce optimal prediction capacity models. R^2 value was used as a statistical measure of prediction performance of the models. R^2 values close to 1 indicate that

the model has high accuracy at predicting the target data set whereas, values below 0.9 were considered insensitive at learning the pattern in the data and that model prediction capacity was not suffice (Baldo et al., 2018). In figures 4a-4d, a point-to-point comparison was further demonstrated between the actual experimental data and model predicted data for all models.



(a) (b)

Figure 4: Comparison between actual and ANN predicted G* and δ



(c) (d)

Figure 4: Comparison between actual and ANN predicted G' and G''

Illustrated in the Figure. 5, R^2 values higher than 0.9 were observed both with training and testing data sets in the three scenarios which were modeled for predicting G*, G' and G''. On

the other hand, the lowest prediction capacity was observed with the model developed for δ prediction.

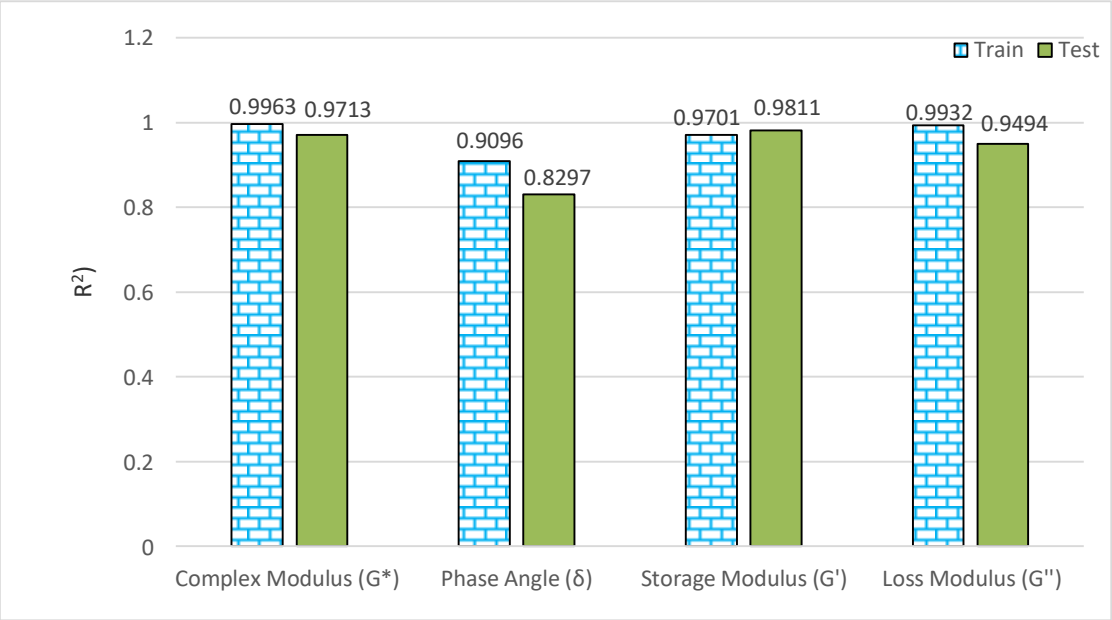


Figure 5: R^2 values for training algorithms

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

Table 2: 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

4. 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 3,5 and 7% addition of geopolymer composed of fly ash and the alkali liquid. Following conclusions can be drawn in this study:

- The best performing model was developed for predicting G*. Features of the model included 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.
- 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 be as precise for predicting untrained datasets.
- Based on R^2 results, the model developed for predicting δ was observed as the least efficient model regarding prediction capacity. R^2 value of 0.823 with the testing dataset revealed that the model was unable to learn complexity in the data and that would perform poorly with untrained new datasets.

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