Research Article

A multi-structure multi-run range (MSMRR) approach for using machine learning with constrained data in pavement engineering

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Abstract
In pavement engineering, the data sets that are typically obtained from experiments are small and cannot be classified as big data. The effective use of machine learning techniques such as artificial neural networks (ANN) for small data is a challenge because of poor accuracy of models. This paper presents a method of multiple structure multiple run and ranging to optimize ANN to produce models with small data sets with high accuracy. In this method, a large number of data fitting ANNs, with different number of neurons, layers, training and validation ratios, and randomized layer weights and biases are run in parallel, and the most accurate ANN is filtered out on the basis of the lowest MSE or highest R. The process is demonstrated with weather and pavement temperature data for a hot mix asphalt (HMA) and an open graded friction course (OGFC) pavement. Models are generated to predict the temperature at a depth of 12.5 mm below the surface. For the HMA pavement, an accuracy of 99.73% was obtained and an optimum structure was found to be with 4 layers, 11 neurons, 70% training ratio, 15% validation ratio. In the case of the OGFC pavement, an accuracy of 99.75% was obtained for an optimum structure with 3 layers, 11 neurons, 75% training ratio, 15% validation ratio. Furthermore, the fitting/regression problem was converted to a classification problem with different ranges, and then ANNs were utilized to develop very accurate classification models with small datasets.

Keywords Machine learning · Artificial neural network · Small data · Regression · Classification · Pavement · Temperature

1 Introduction

Analysis of data is critical for material characterization, and building constitutive and predictive models in pavement engineering. To date, most of the analyses in pavement engineering are conducted with conventional statistical methods. This approach makes several assumptions such as linearity, independent inputs and normal residuals, which in many cases may not be true for the data. Machine learning (ML) can help researchers overcome such problems, and techniques such as artificial neural networks (ANNs) are particularly helpful in prediction and/or classification in the case of data with high degree of non-linearity, complex boundaries and with many dimensions or features (predictors). Furthermore, the accuracy of properly trained ANNs have been demonstrated to be much greater than that of statistical or empirical models [1]. Soft computing methods such as neuro-fuzzy models and ANN have been used to predict shear capacity and compressive strength of concrete structures with high accuracy [2, 3]. A literature review indicates examples of application of the use of ANNs in a variety of cases for pavement engineering such as for predicting moduli from falling weight deflectometer (FWD) testing [4–6], spectral analysis of surface waves [7], prediction of laboratory permeability of hot mix asphalt (HMA) [8] and pavement performance [9–11], estimation of laboratory dynamic modulus of HMA [12, 13] and pavement temperatures [14], prediction of non-linear

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material response [15], in-place layer moduli [16], foaming qualities of mixers [17], moisture damage of modified binders [18], field permeability of asphalt pavements [19] and in pavement management [20]. Ceylan et al. [21] has summarized the application of ANN in pavement engineering in the following areas: "(1) prediction of pavement condition and performance, (2) pavement management and maintenance strategies, (3) pavement distress forecasting, (4) structural evaluation of pavement systems, (5) pavement image analysis and classification, (6) pavement materials modeling, and (7) other miscellaneous transportation infrastructure applications."

However, the biggest drawback of using ML is that the effective use of the most commonly used ML method, ANN, requires the use of a significant amount of data. In fact, most, if not almost all of the developments and applications have been for "Big Data" which typically consists of relatively large datasets, with thousands of observations. These data are generally used for identifying associations between parameters, and pattern and trends in behaviors [22, 23]. Unfortunately, in pavement engineering, the data that are available from most laboratory or field experimental studies consist of relatively small or "constrained" data sets, and cannot be classified as "Big Data". This is because experiments in pavement engineering are labor- and time-intensive, and costly. The application of extensive amount of instrumentation/sensor networks is costly, and may be possible only for a few pooled or nationally funded studies. This means that pavement engineers cannot avail the benefits of ANN with most of their data. A similar concern has been recognized in the medical sciences [24–27].

1.1 Problem statement

Despite their tremendous success, ANNs have been strictly restricted in pavement engineering for only those relatively few cases where big data exists, such as those from the Long Term Pavement Performance (LTPP) Study in the US (Infopave, https://infopave.fhwa.dot.gov/). These studies are few in number because of their significant costs. On the other hand, there are several reasons that prevent researchers from applying ANN to solve problems with small datasets. The primary reasons, which affect the ability of a ANN to reach convergence to an objective function (cost function) and produce repeatable results, are the following: (1) ANNs consist of parameters that are randomly initiated, and big datasets are needed to avoid prediction variabilities, and achieve stable behavior; (2) dependence of the results on the training and validation data, and (3) the need for sufficient data points for developing the parameters for fitting highly nonlinear and complex models.

1.2 Objective

The objective of this paper is to present a method that could be utilized to apply artificial neural network (ANN) as a machine learning (ML) technique to develop sufficiently accurate results from analyses of relatively small data sets, which are frequently encountered in the field of pavement engineering.

2 Artificial neural network (ANN)

The structure of an ANN consists of one or more layers of neurons (input, hidden and output layers) through which the input is processed and the outputs are obtained at the end. The structure and the process mimic the biological neural process that is responsible for all brain functions [28, 29]. The process of transmitting the inputs through the layers is manipulated through the use of appropriate layer weights and biases, which dictate the impact of one layer of neurons on the other. The basic process of training an ANN for supervised learning (fitting or classification) consists of iteratively altering the layer weights until an object function such as error between the target value and the predicted value is minimized. The training process can be conducted through various algorithms such as the Levenberg–Marquardt (LM) algorithm [30, 31] or the Bayesian regularization technique [32]. Typically, the dataset is divided into training, validation and test ratios. The training dataset is used to develop the model, which is tested with the validation dataset to ensure the accuracy and then further checked with the test dataset. The checking can be done with various parameters—but typically the mean square error (MSE) and the coefficient of correlation (R) are used for fitting, whereas a confusion matrix is used for classification.

2.1 Example of a relevant pavement engineering problem

The authors have selected the prediction of temperatures at different pavement depths from weather data as a relevant problem for this paper. The topic has been a subject of interest and research for a number of years, since such prediction is crucial for the selection of the appropriate stiffness/strength properties (such as dynamic modulus) of pavement materials, which are used for prediction of pavement performance through mechanistic or mechanistic-empirical modeling and analysis. Over the last few decades, a number of researchers have carried out investigations on predicting maximum temperatures and temperature at different depths of pavement layers from weather data (for example, [33–39]), and a number of statistical models are available in the literature. Some researchers have also used ANN for prediction of pavement temperatures; Abo-Hashema [14] and Matić et al. [40] have used data from LTPP and that from a year-long study at a University campus, respectively. Researchers of both studies have reported excellent accuracy in prediction of pavement temperatures using ANN.

Although researchers have used different types of predictors, such as surface temperatures, the quest through the different years has always been for the ability to predict the temperature at a relevant pavement depth from the data that could be obtained easily. However, it is also true that the pavement temperature at the surface and at different depths are dependent on a number of weather factors as well as thermodynamic properties such as heat capacity and conductivity, and on the thermal history of the location. On the basis of the above considerations, and the availability of data, the authors had selected the following relevant predictors for analyses from two different types of pavement sections, a dense graded hot mix asphalt (HMA) and an open graded friction course (OGFC): solar radiation, wind speed, air temperature, rainfall and surface temperature. Additionally, following the work of Abo-Hashema [14] the authors also calculated and used the thermal history (average air temperature from 24 h preceding the time of testing) as one of the predictors in the ANN model. The temperature at a depth of 12.5 mm was selected as the target parameter.

3 Methodology

In this paper, the use of a multi-structure-multi-run range (MSMRR) approach is proposed, demonstrated and evaluated for the effective use of ANN for fitting and classification with small data. The basis of this approach is the hypothesis that multiple runs with multiple structures, initial weights, and bias of layers with ANN, and grouping of targets into data ranges and predicting ranges rather than exact values can yield sufficiently accurate results from the analysis of small datasets compared to those from analysis with larger datasets. The analysis has been carried out using small and large data sets.

The approach consists of using multiple structures (different number of neurons and layers) in ANN and running them multiple times [27], while initializing the weights and biases every time, to come up with combination of various ANNs, from which the best structure (lowest MSE) is identified. Furthermore, the targets in different runs were grouped into different ranges, starting from narrow to broad. Statistical tests were conducted between the results of the different runs to determine significant differences in the results if any. The results from the analysis of the smaller datasets were compared against those from analyses of the entire dataset, to detect differences in accuracy, if any, and hence determine the loss in accuracy of prediction for using smaller datasets. Finally, an optimum MSMRR method was proposed that could be used with relatively smaller datasets.

4 Data and analysis

For this paper, the two datasets corresponding to the two pavement sections, consisting of weather data and pavement surface temperature, and the temperature at a depth of 12.5 mm below the surface, were utilized. The sections consisted of 100 mm HMA and 100 mm OGFC layers over 150 mm and 300 mm of aggregate base, respectively over the same existing soil subgrade. The data were collected from a year-long study at the UC Davis Pavement Research Center as part of a bigger study [41]. Each dataset consists of 8000 observations of solar radiation (SR), wind speed (WS), rainfall (RF), air temperature (AT), thermal history (TH) and surface temperature (ST) (predictors), and the temperature at a depth of 12.5 mm (target). A small portion of the data is shown in Table 1 as example. The maximum and minimum values for the data are shown in Table 2. The weather data were obtained from weather stations with different sensors on each of the two test sections, while the pavement temperature data were obtained from thermocouples installed at the surface and different depths.

4.1 Use of artificial neural network (ANN)

A higher number of observations (that are used for training the model) has been always found to result in better (more accurate) ANN models. In addition, techniques such as early stopping and k-fold cross validations are generally used for avoiding overfitting. The hypothesis adopted in this study is that the impact of the relative differences (sometimes referred to as volatilities) between the ANNs with different properties for small data sets could be reduced by running multiple structures multiple times. Multiple structures refer to multiple layers and different number of neurons in the layer. Furthermore, the layer weights and biases are initialized randomly according to the Nguyen–Widrow [42] algorithm, which distributes the active region of each neuron in the layer evenly across the layer's input space and reduces the wastage of neurons. This algorithm is widely used to increase the accuracy of ANN network [43, 44]. Lastly, the training and validation ratios of the total dataset were also varied. These

Table 1 Example of temperature and weather data

Observations (at 30 min interval)	Air temperature (°C)	Solar radiation (W/m^2)	Rainfall (mm)	Wind speed (m/s)	Surface temperature (°C)	Temperature at a depth of 12.5 mm (°C)
HMA						
1	8.9	0	0.0	1.3	15.5	15.3
2	8.6	2	0.0	1.0	15.3	15.1
3	10.1	36	0.0	1.2	15.8	15.5
4	11.0	128	0.0	0.9	16.5	16.0
5	12.4	252	0.0	1.9	20.6	19.0
OGFC						
1	9.3	0	0.0	0.6	12.13	14.82
2	9.3	0	0.0	0.4	11.78	14.51
3	10.2	9	0.0	0.3	12.4	14.71
4	12.8	98	0.0	0.8	13.15	15.13
5	13.0	192	0.0	0.5	15.48	15.48

Table 2 Maximum and minimum parameters for OGHC and HMA pavement data

Sample	Parameter	ST	AT	SR	RF	WS	TH	$T_{12.5}$
OGFC	Maximum	67.48	40	1420	6.35	12.9	40.27	62.9
	Minimum	−6.322	−7.6	0	0	0.278	−38.71	−3.879
	Total	8000						
HMA	Maximum	71.5	41.01	1292	9.91	12.29	46.93	59.46
	Minimum	−1.701	−4.781	0	0	0.278	−40.78	−0.894
	Total	8000						

parameters have been found to be very significant in affecting the performance of ANNs specifically for cases with relatively small data sets and recommendations have been made for using multiple splits (as opposed to a single split) of the data for the development of ANN models [45]. Finally, the algorithm used to generate the ANNs included a step for filtering out the optimum ANN, based on minimum MSE and maximum R. The algorithm is shown schematically in Fig. 1. All analyses were conducted using MATLAB® software [46].

4.2 Impact of number of observations

First, the impacts of the amount of data on MSE and R were evaluated by running ANNs with different structures and number of neurons and by initializing the weights and biases randomly in each run, for multiple runs. The ANN parameters that were varied for different simulations are shown in Table 3. The reduced data sets (from a total of 8000 observations) consisted of 1000, 500 and 100 observations, all of which were selected randomly from the entire data set.

A total of 1800 runs were conducted for the different combinations. The MSE and R values obtained for each amount of data were compared using the Mann–Whitney test (which compares the median values). The

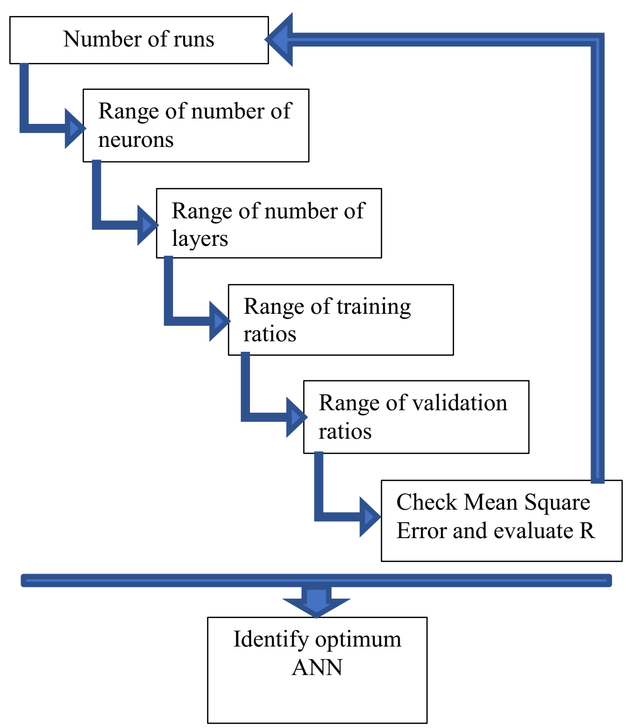


Fig. 1 Schematic flowchart of the ANN algorithm

Table 3 Dataset and ANN parameters

Parameter	Values
Data (rows of observations)	8000; 1000; 500; 100
No. of neurons in hidden layers	3, 5, 7, 9, 11
Percent of training data	70, 75, 80
Percent of validation data	15, 10
Number of hidden layers	2, 3, 4
Number of runs[a]	5

[a]Each run corresponds to an initialized random set of layer weights and bias; Z-score normalization has been considered; single layer ANN did not show any reduction in MSE

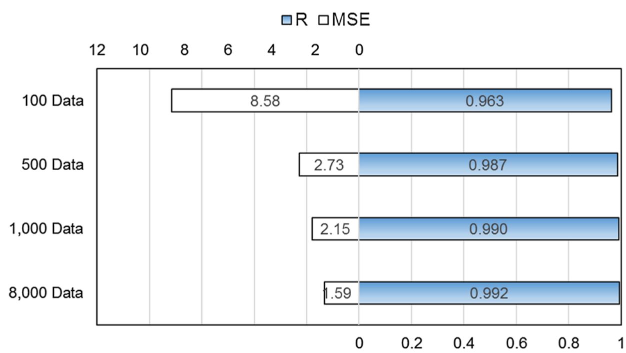


Fig. 2 Median R and MSE values for the different datasets (HMA pavement)

results indicated relatively lower R and higher MSE values for the models with the smaller data sets (Fig. 2).

As expected, the MSE increased and the R value dropped progressively from the model with 8000 data points to the model with 100 data points, although the R value for the 100 data points model was still found to be quite high (0.963). An Analysis of Variance (ANOVA) showed a significant effect on the R value [F(6,1793) = 8.69, $p < 0.0001$] but insignificant effect on the MSE value [(F(6,1793) = 1.05, $p = 0.39$. However, a regression analysis did not yield meaningful results ($R^2 = 0.03$), which indicates that the impact of the different parameters on the MSE and R of the different models cannot be explained with a generalized linear model. In fact, the impact of the parameters such as number of neurons on the performance of ANN models is not well understood, and the trial rule has been the most widely used method [47]. This effectively means that although one knows the significant impacts, it is not possible to draw a conclusion regarding the optimization of the different parameters in the ANN.

4.3 Multiple run multiple structure and ranging (MSMRR)

To overcome this problem, the method of multiple run multiple structure and ranging (MSMRR) is proposed. In this method, the small data set is used for running multiple ANNs in parallel using the different parameters listed in Table 3. Next, the optimal structure is extracted from the runs on the basis of the highest R value. For the HMA pavement data, this technique was applied on the 100-sample dataset and the best structure was identified as one, which gave the high test R value of 0.99. The optimum ANN was found to be with three layers, 9 neurons, 80% training ratio, 15% validation ratio. The technique was also applied for the OGFC pavement data and the optimum ANN was found to be with three layers, 5 neurons, 80% training ratio, 15% validation ratio (R = 0.99). Figure 3a, b show the optimum structures of the prediction models for HMA and OGFC pavements, including layer weights and biases.

Comparisons between the predicted and the actual values for the two pavements are shown in Fig. 4. It can be seen that a high R value is obtained for the prediction of the temperature at a depth of 12.5 mm for both HMA and OGFC pavements.

5 Results and discussion

Note that while an accurate prediction of temperatures is desirable, the accuracy that is required is dependent on the sensitivity of the critical performance based property to temperature. For example, research data shows that the dynamic modulus (a critical property that is utilized for prediction of strain in the HMA layers in the mechanistic-empirical analysis and design of asphalt pavements, AASHTO [48] values of HMA exhibit distinct sets of values at five different temperature ranges: > 30 °C, 20–30 °C, 10–20 °C, 0–10 °C and < 0 °C. At both extremes of temperature (high and low) the dynamic modulus values tend to level off. At lower temperatures, beyond a certain level, the change in calculated critical strain becomes practically insensitive to further changes in the dynamic modulus (because of a relatively high dynamic modulus), while beyond a certain high temperature, the dynamic modulus values are typically very low, and correspondingly, extremely high strain values are expected. The shorter the temperature range of the location, the less number of ranges need to be specified. For example, in the case of the current data set from Davis, California, USA, the lowest temperature that was recorded was – 1 °C, and the range need not extend beyond that temperature. For a region with a wide range of temperature, the number of ranges

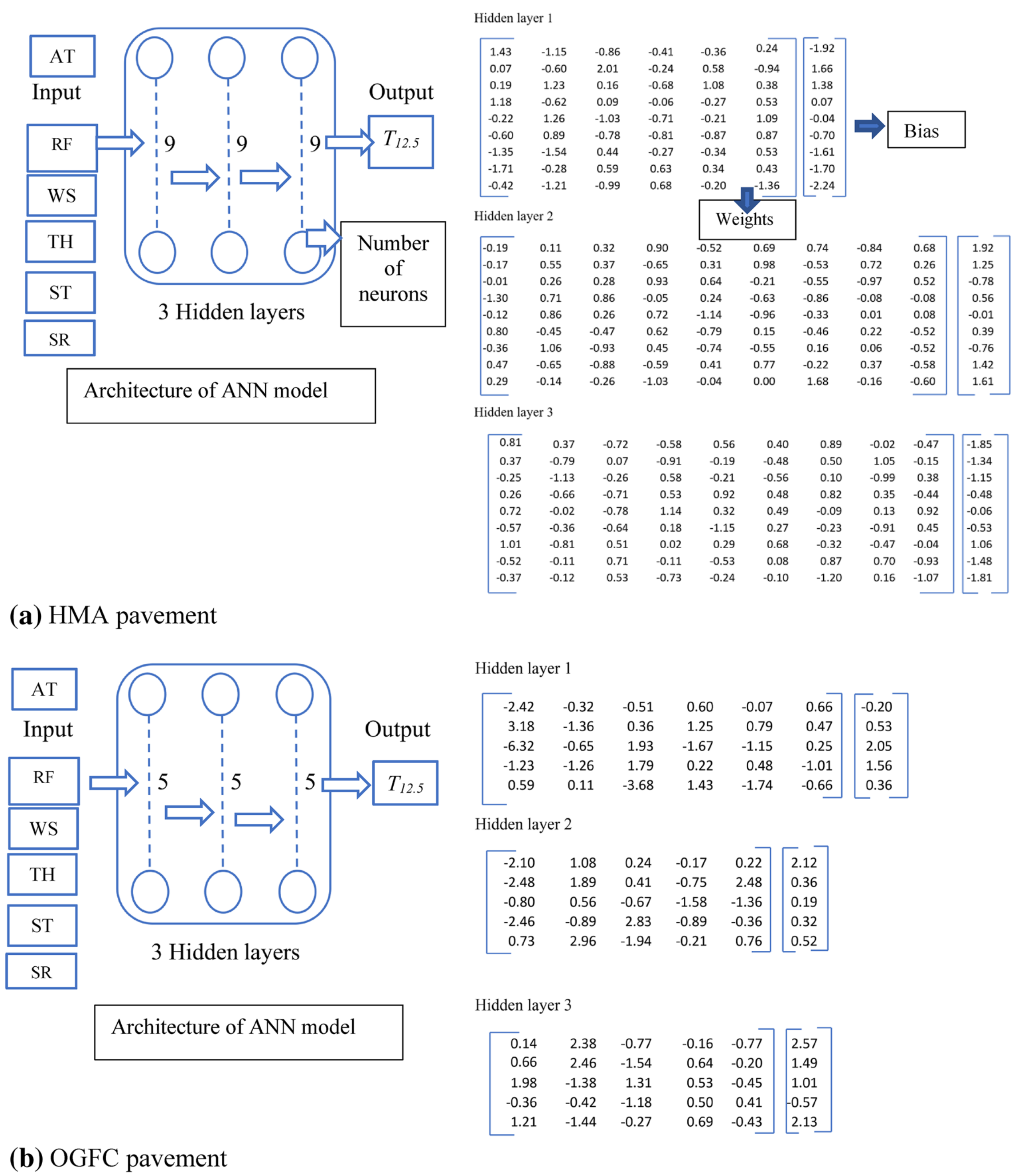
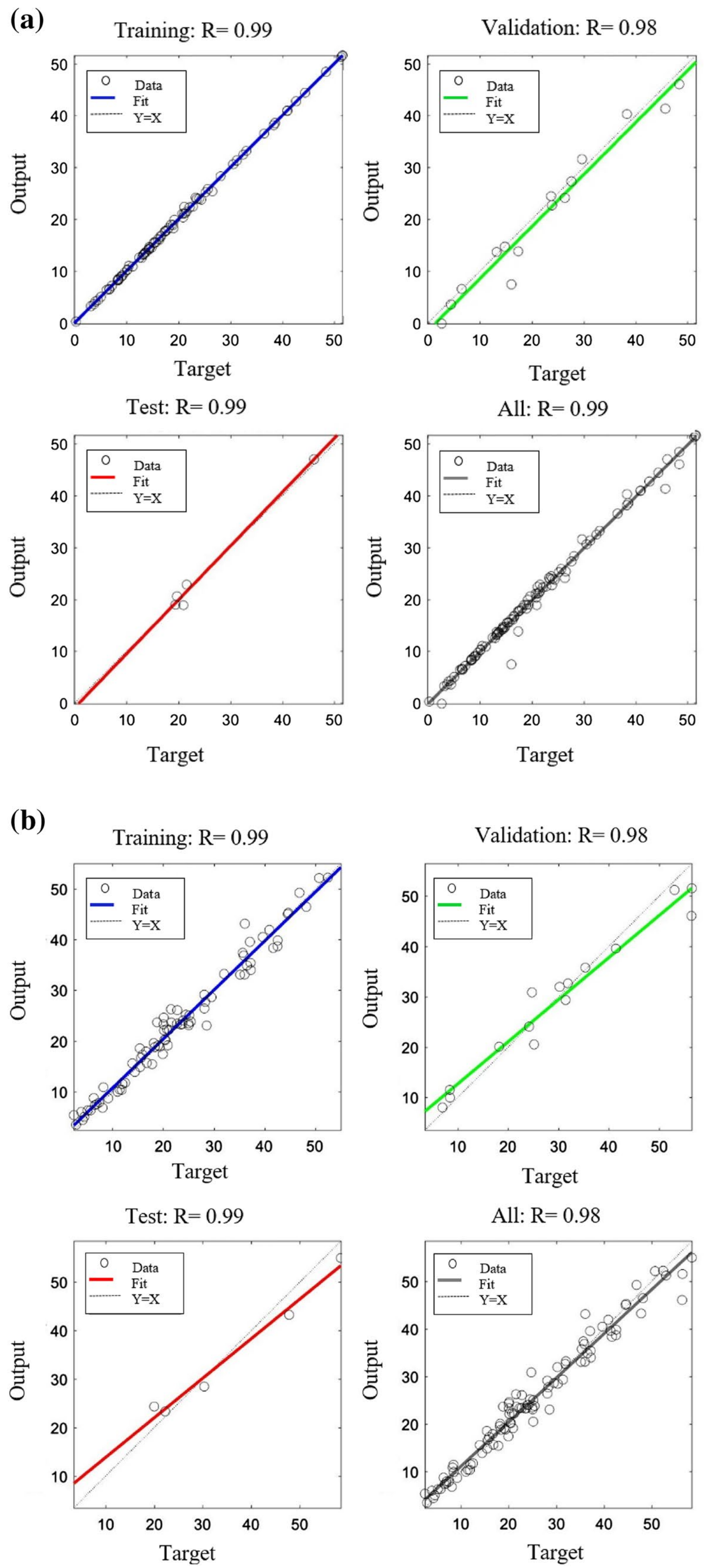


Fig. 3 Optimum structures of prediction models of HMA and OGFC temperatures. *Note*: Inputs are solar radiation (SR), wind speed (WS), rainfall (RF), air temperature (AT), thermal history (TH) and surface temperature (ST); output is $T_{12.5}$ temperature at a depth of 12.5 mm

can be relatively large, such as ten. What is important here is to note that instead of trying to predict whether the temperature is either one of the 30 values ranging from say 0 to 30 °C (at 1-degree interval), it may be sufficient to predict to which of the three or ten ranges it belongs to. Prediction of temperature of a HMA layer at one of those ranges will be sufficient for the selection of the appropriate dynamic modulus values. The advantage is that a reduction in number of targets or "bins" by effectively using ranges (and broader ranges) instead of actual values can enable us to use ANNs that work well with a relatively small dataset. To give a similar example, one needs a small number of data to fit a simple curve (say a quadratic polynomial) and a relatively large number of data points to fit a more complex curve (say a sine wave).

To evaluate the impact of ranging, the HMA and the OGFC pavement data were divided into different intervals, and the 100 observations data set was utilized for

Fig. 4 Plots of actual versus predicted temperatures for **a** HMA, **b** OGFC pavement



the training of the ANN. The data was grouped as narrow range, broad range and very broad range. Narrow range had five groups: very low (< 9 °C), low (10–19 °C), medium (20–29 °C), high (30–39 °C) and very high (> 40 °C). The broad range consisted of low (< 15 °C), medium (16–30 °C), high (31–45 °C) and very high (> 46 °C) groups. The very broad range had low (< 19 °C), medium (20–39 °C) and high (> 40 °C) groups. Although the 100 observations were selected randomly, it was made sure that the data was well balanced in terms of all of the ranges. In practice, it is expected that if one has 100 data points to begin with, the ranges will be well represented in the data. The ANN was then trained as a classification net, using Levenberg–Marquardt algorithm. The number of layers and neurons were varied according to the range presented in Table 3. For the HMA this technique was applied on the 100 sample dataset and the best structure was identified as one which gave the lowest test error percentage of 0.27% (Accuracy 99.73%). The optimum structure was found to be with 4 layers, 11 neurons, 70% training ratio, 15% validation ratio. The technique was also applied for the OGFC pavement data and the optimal structure was found to be with 3 layers, 11 neurons, 75% training ratio, 15% validation ratio, with the lowest test error percentage of 0.25% (accuracy of 99.75%). The optimum networks and error rates for the different ranges from classification models are presented in Table 4.

6 Summary and conclusions

The use of machine learning (ML) techniques provides a significantly better method of analysis compared to conventional statistical methods, specifically for complex and highly non-linear data. However, the use of the most common machine learning (ML) technique, artificial neural networks (ANN) for analysis of small data sets is challenging because of poor accuracy and repeatability. Due to time and budget limitations, most data sets that are obtained from pavement engineering experiments are relatively small and cannot be classified as Big Data. To overcome the volatility of results of ANN using small datasets, a method of multiple structure multiple run and ranging (MSMRR) is proposed and demonstrated in this paper. The multiple runs and multiple structures, along with randomly generated layer weights and biases were used with a filtering algorithm to select the best ANN on the basis of a governing criterion of global minimum mean square error (MSE). A method of changing an appropriate small-data problem from a fitting to a classification analysis was also proposed. The method was demonstrated with an example of prediction of pavement subsurface temperature from weather and pavement surface data.

The following conclusions are made from this study.

1. The multiple structure multiple run and ranging (MSMRR) method is capable of producing ANN models with good accuracy for small data sets.
2. Models with good accuracies can be developed from small datasets by transforming fitting problems to appropriate classification problems.

Table 4 Optimum networks and error rates for the different ranges from classification models

Group	HMA data	Number of runs	Number of neurons	Number of layers	Training ratio	Validation ratio	Error rate
Broad	Overall	2	9	2	0.8	0.15	0.0030
	Test	2	7	2	0.8	0.15	0.0046
Narrow	Overall	5	11	3	0.7	0.15	0.0193
	Test	1	11	2	0.8	0.15	0.0202
Very broad	Overall	3	5	4	0.8	0.1	0.0013
	Test	5	11	4	0.7	0.15	0.0027
Group	OGFC data	Number of runs	Number of neurons	Number of layers	Training ratio	Validation ratio	Error rate
Broad	Overall	5	5	2	0.8	0.15	0.0049
	Test	1	7	2	0.8	0.15	0.0062
Narrow	Overall	2	5	2	0.8	0.1	0.0155
	Test	5	7	2	0.8	0.15	0.0249
Very broad	Overall	5	7	2	0.8	0.1	2.32×10^{-6}
	Test	2	11	3	0.75	0.15	0.0025

3. A combined use of MSMRR and classification problems can be made successfully in pavement engineering to utilize ANN to develop accurate prediction models with small datasets.

Compliance with ethical standards

Conflict of interest On behalf of all authors, the corresponding author states that there is no conflict of interest.

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