IJESRT

INTERNATIONAL JOURNAL OF ENGINEERING SCIENCES & RESEARCH TECHNOLOGY

Numerical Study of Back Propagation Learning Algorithms for Forecasting Water Quality Index

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Abstract

Artificial intelligence techniques, such as neural networks are modeling tools that can be applied to predict water quality parameters. Artificial neural networks are frequently used to model various highly variable and nonlinear physical phenomena in the water and environmental engineering fields. This article describes design and application of feed-forward, fully-connected, three-layer perceptron neural network model for computing the water quality index (WQI) for Batlagundu, Dindigul District, Tamilnadu. The modeling efforts showed that the optimal network architecture was 8-3-1 and that the best WQI predictions were associated with the back propagation (BP) algorithm. The WQI predictions of this model had significant, positive, very high correlation with the measured WQI values, implying that the model predictions explain around 95.4% of the variation in the measured WQI values. The approach presented in this article offers useful and powerful alternative to WQI computation and prediction, especially in the case of WQI calculation methods which involve lengthy computations and use of various sub-index formulae for each value or range of values of the constituent water quality variables.

Keywords : Artificial intelligence, Three-layer perceptron, Back propagation, correlation coefficient, WQI

Introduction

India is endowed with rich and vast diversity of natural resources, water being one of them. Water is nature's most wonderful, abundant and useful compound. Of the many essential elements for the existence of human being, animal and plant, water is rated to be of the greatest importance. Groundwater is an important source of water supply throughout the world. It is well known fact that potable safe water is absolutely essential for healthy living. Adequate supply of fresh and safe drinking water is the basic need for all human beings on earth. Anthropogenic activities can impact negatively on the water quality of the freshwater bodies thereby limiting their scope of usage. The problem of drinking water contamination, water conservation and water quality management has assumed a very complex shape. Groundwater quality assessment is a part of environment assessment and groundwater quality is closely related with human health.

The water quality is normally assessed by measuring a broad range of parameters such as temperature, pH, electric conductivity (EC), turbidity and the concentrations of a variety of pollutants including pathogens, nutrients, organics and metals. In consequence, a large amount of data is generated by the monitoring programs and these data require integration if the monitoring results are to be presented in a meaningful way to local planners and decision makers, watershed managers, and the general public. In view of this, water quality indices have been developed to integrate measurements of a set of parameters into a single index (Zandbergen and Hall, 1998). A quality index is a unit less number that assigns a quality value to an aggregate set of measured parameters (Pesce and Wunderlin, 2000). So, the water quality index (WQI) may be defined as a single numeric score that describes the water quality condition at a particular location in a specific time (Kaurish and Younos, 2007).In natural environment, water quality is a multivariate phenomenon, at least as reflected in the multitude of constituents which are used to characterize the quality of water body.

It is very important to evaluate the contribution of each parameter used in calculation of WQI. The calculation of such WQIs takes time and effort and may be occasionally associated with

ISSN: 2277-9655
Impact Factor: 1.852

unintentional errors during sub-index calculations. This argument is not in any way intended to undermine or undervalue these indices which are well-established and which being founded on solid scientific grounds and are proved to be highly successful and effective in practice. Rather, an alternative, direct and quick means of computing and forecasting WQI values based on artificial neural network (ANN) modeling that has the potential to reduce the computation time and effort and the possibility of errors in the calculation is suggested. Therefore, this study illustrates design of a neural network model for rapid, direct calculation of the WQI as an alternative to WQI computation methods involving sub-indexing and lengthy calculations. The ANNs are popular tools for modeling highly complicated relationships, processes and phenomena.

The main objectives of this study were to (i) demonstrate the potential of the ANN for producing models capable of efficient forecasting of the WQI; (ii) illustrate the general framework for ANN model design (e.g., selection of network type; determination of appropriate input variables and number of hidden neurons; and specification of the optimum settings of the network training parameters); and (iii) establish a neural network model that can be used to directly foresee the water quality status of the study area and thus provide a reliable alternative to the WQI calculation method currently in use.

Materials and Methods

Study Area

The study area Batlagundu is bounded by Longitude 77 ^{0} 45' 33.84" E and Latitude is 10 ^{0} 9' 55.80" N with an average elevation of 320 meters (1049 feet). The main occupation of this study area is agriculture. The sources of water supply in the area are hand pumps, bore holes and dug wells. The precipitation which is the sole source of ground water recharges in the study area is very low. The area is very humid (86%) and warm with an average temperature 22 ^{0}C. In order to achieve the research objective, samples were collected from 18 sample points on a monthly basis from 2012 to 2013. This dataset comprised 3600 data points derived from 24 measurements on 150 samples. The 24 water quality variables are temperature, pH, sulphate, potassium, phosphate, turbidity, total dissolved solids, electrical conductivity, total hardness, total alkalinity, calcium, magnesium, chloride, nitrate, nitrite, fluoride, sodium, iron, ammonia Dissolved Oxygen, Biochemical Oxygen Demand and Chemical Oxygen Demand. However, not all water quality variables were employed in the study. The variables were examined for their effects on the water quality of study area using correlation analysis which reduced this number to 8 variables. Subsequently, only these 8 water quality variables such as pH, dissolved oxygen(DO), total dissolved solids(TDS), electrical conductivity(EC), total hardness, calcium (Ca) ions, magnesium(Mg)ions, and total alkalinity were employed in the ANN modeling. Values of some descriptive statistics for these variables are shown in Table 1. Fig.1 shows the map of the study area.

Calculation of Water Quality Index

Water quality index was calculated for assessing the suitability of water for biotic communities and also drinking purposes. It was done by considering eight important physico chemical properties using Central Public Health Environmental Engineering Organization (CPHEEO), 1991 & Indian Council of Medical Research (ICMR) 1975 standards.

In order to calculate WQI eight important parameters namely pH, dissolved oxygen(DO), total dissolved solids(TDS), electrical conductivity(EC), total hardness, calcium (Ca) ions, magnesium(Mg)ions, and total alkalinity have been selected. For the calculation water quality index, the weightage of each factor is given in Table 2. Factors which have higher permissible limits are less harmful because they can harm quality of ground water when they are present in very high quality. So weightage of factor has an inverse relationship with its permissible limits.

$$W_i \propto \frac{1}{V_i} \quad \text{or}$$

$$W_i = \frac{k}{V_i} \quad \ldots\ldots\ldots\ldots\ldots\ldots \text{(1)}$$

Where

k= constant of proportionality

W_i= unit weight factor

V_i= maximum permissible limits as recommended by Indian council of Medical Research/ Public Health Environmental engineering Organization.

Value of k was calculated as

$$k = \frac{1}{\sum_{i=1}^{8} \frac{1}{V_i}} \quad \ldots\ldots\ldots\ldots\ldots \text{(2)}$$

Where

$$\sum_{i=1}^{8} \frac{1}{V_i} = \frac{1}{V_{i(pH)}} + \frac{1}{V_{i(TDS)}} + \frac{1}{V_{i(Hardness)}} + \frac{1}{V_{i(Ca)}} + \frac{1}{V_{i(Mg)}} + \frac{1}{V_{i(Total\ Alkalinity)}} + \frac{1}{V_{i(DO)}} + \frac{1}{V_{i(EC)}} \text{---(3)}$$

The weightage of all the chemical factors were calculated on the basis of this equation.

$$WQI = Wi\ x\ Vr \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(4)}$$

i.e., Water Quality Index is equal to the product of rating (Vr) and unit weight (Wi) of all the factors.

$$W_i \times V_r = W_{i(pH)} \times V_{r(pH)} + W_{i(TDS)} \times V_{r(TDS)} + W_{i(Hardness)} \times V_{r(Hardness)} + W_{i(Ca)} \times V_{r(Ca)} + W_{i(Mg)} \times V_{r(Mg)} + W_{i(Total\ Alkalinity)} \times V_{r(Total\ Alkalinity)} + W_{i\ (DO)} \times V_{r\ (DO)} + W_{i\ (EC)} \times V_{r\ (EC)} \quad \ldots\ldots\ldots\ldots\ldots (5)$$

The values of V_i, W_i, and V_r are given in Tables 2 and Table 3. Hence by multiplying W_i and V_r value of WQI is calculated. Based on the calculated WQI, the water quality may be classified as four classes by Tiwari and Misra (1985). This computed value of WQI, which served as the dependent variable in the WQI – ANN model is developed in the study.

Development of the ANN model

The ANNs represent an innovative and attractive solution to the problem of relating output variables to input ones in complex systems (Dawson and Wilby, 2001) and prediction is a common reason for employment of the neural network technology. The major steps for development of ANN models include defining the suitable model inputs, specifying network type, pre-processing and partitioning of the available data; determining network architecture; defining model performance criteria; training (optimization of connection weights); and validating the model (Dawson and Wilby, 2001; Govindaraju, 2000; Maier and Dandy, 2000). These steps are outlined below.

Optimization of network architecture

This study employed a parallel, feed-forward, fully-connected, multilayer perceptron (MLP) neural network in order to establish a non-linear regression model that can be used to directly foresee the water quality status of study area, in terms of the WQI, using water quality monitoring data. Construction of this model was carried out in two major steps; determination of the network architecture and specification of the network structure. The first step aimed at determining the numbers of input, hidden, and output layers; the numbers of input, hidden, and output neurons; and the optimal data splitting plan. While the second phase involved specifying the training algorithm, learning rate, number of iterations, number of retrains and training stopping criteria.

The hidden layers provide the network with its ability to generalize. In theory, a network with a hidden layer and adequate number of hidden neurons can simulate any continuous function and represents a rich and flexible class of universal approximators (Dawson and Wilby, 2001; Palani et al., 2008). Thereupon, this study employed a neural network with one input layer, one hidden layer, and the WQI as the output layer, thus producing a three-layer perceptron (TLP) network. Empirical datasets usually have variables of different measurement units and are quite often burdened with some measurement errors, noise, or interference. These factors may exert negative impacts on operation of some ANN training algorithms. In order to avoid such impacts it is necessary during the initial data preparation stage to standardize the data, that is, to convert the data into a non-dimensional form of uniform range of variability (Dawson and Wilby, 2001; Ozesmi et al., 2006). This prevents any attribute from arbitrarily dominating the neural network modeling outputs. Hence, the input water quality data were pre-processed by standardization within the limits of the logistic sigmoid function, i.e., 0–1.

The number of water samples (or examples) available for modeling was 150 and the number of input water quality variables (neurons) was 8. The 150 samples were divided into training, validation (or over-fitting), and testing sets. The testing subset should include data never used in the training and cross-validation sets and this data should constitute approximately 10–40% of the size of the training set (Palani et al., 2008). The number of input and output units is usually fixed, depending on the number of input predictors and output variables (Bruzzone et al., 2004). However, determining the number of hidden nodes is usually a trial and error task in ANN modeling (Ozesmi et al., 2006; Palani et al., 2008; Singh et al., 2009). There is no magic formula for the selection but there are some rules of thumb. As an example, Fletcher and Goss (1993) stated that the appropriate number of neurons in the hidden layer (N_h) ranges from $2I^{1/2} + O$ to $2I + 1$, where I and O represent the numbers of input and output nodes, respectively. The Alyuda Research Company (2003) however maintains that N_h should fall within the range of I/2 to 4I. More recently, Palani et al. (2008) supported that N_h can lie between I and 2I + 1 and that it should not in any way be less than the maximum of I/3 and O. However, networks with few hidden nodes are generally preferable to networks with many hidden nodes because the former usually have better generalization capabilities and fewer over-fitting problems than the latter (Khalil et al., 2011; Ozesmi et al., 2006; Palani et al., 2008). In the current case, I is 8 and O is 1. Therefore, the typical number of hidden nodes is expected to be $\geq 8/3 \approx 3$ neurons and $\leq 8 \times 4 = 32$ neurons ($3 \leq N_h \leq 32$). Within this range, the most suitable value of N_h was determined following the trial and error approach.

As activation of the neurons, the sigmoidal-type (logistic sigmoid and hyperbolic tangent) functions and the Gaussian function are non-linear activation functions that can be used in the MLP neural networks. However, the logistic sigmoid and hyperbolic tangent functions are the functions most commonly used with the MLP neural networks (Dawson and Wilby, 2001; Maier and Dandy, 2000) while the Gaussian function is the one most commonly used with the RBF neural networks (Corsini et al., 2003; Dawson and Wilby, 2001). The logistic sigmoid function is particularly appealing when the raw data have outliers because this function reduces the effects of extreme input values on the performance of the network and hence extreme values will have no extreme effects on the network outputs (Hill et al., 1994). Consequently, this study used a linear transfer function in the input layer and a logistic sigmoid activation function in the hidden and output layers.

Eventually, this search process showed that the optimal network architecture was 8-3-1 and that the optimum associated partitioning scheme was 70%-15%-15% (i.e., the proportions of the samples allocated to the training, validation, and testing sets were 70%, 15%, and 15%, respectively). In light of the findings related to the best network architecture, the water quality data were divided into a training subset made-up of 104 samples (70% of the samples) and cross-validation and testing subsets comprising 23 samples each (15% of the samples). Fig.2 shows the optimal network architecture of the study.

Model selection, performance and evaluation

Usually either of two broad types of model selection approaches is followed in ANN modeling. The first is the cross-validation-based approach whereas the second is the in-sample model selection method. The cross-validation-based approach divides the available data into three sets: training, validation (or cross-validation), and testing sets. The training set is employed in training the network while the cross-validation set is used for deciding on when to stop training before over-fitting takes place and it is assumed that a good model is a model that minimizes the cross-validation error (Liao and Fildes, 2005; Qi and Zhang, 2001; Turney, 1993). On the other hand, the testing set is utilized for genuine out-of-sample evaluation (Qi and Zhang, 2001), i.e., for estimating the network performance after training has finished, and the true network error is then estimated as the testing set error (Qi and Zhang, 2001; Twomey and Smith, 1998). If representative training data is used, the testing set error is an optimal estimation of the actual network performance (Liao and Fildes, 2005; Prechelt, 1998; Turney, 1993). So, the training set is used for parameter estimation for a number of alternative neural network specifications (e.g., networks of different numbers of inputs and different numbers of hidden layer units). Then, the trained network is evaluated with the validation set and the network model that performs the best on the validation set is selected as the final forecasting model. Thereafter, the validity, usefulness, and generalization performance of the model is evaluated on the testing set (Prechelt, 1998; Qi and Zhang, 2001) using a suitable performance measure like mean square error. In addition to the foregoing error measures, Flavelle (1992) supported that linear regression analysis of the model predictions and the measured data can be used to evaluate the results of a validation in an objective and quantitative manner. According to this approach, the coefficient of correlation is a measure of goodness-of-fit of the model to the data that represents the model's predictive capacity.

Therefore, this study differentiated between the different potential ANN models based on the (i) Mean square error and (ii) correlation between the predicted and observed WQI values (Fox, 1981; Miao et al., 2006) Thus, the ANN model reported here is the model which exhibited the lowest error ; highest correlation between the predicted and observed WQI values.

Results and Discussion

This study employed a parallel, fully-connected, feed-forward MLP network with one input layer, one hidden layer and the WQI as the output layer. The number of examples available for modeling was 150. The numbers of neurons in the input and output layers were fixed to 8 (the number of input water quality variables) and 1 (the WQI) respectively. The input water quality data were pre-processed by standardization to the range of (0, 1). Afterwards, a search for the optimal network architecture and best data partitioning scheme was conducted using the nftool in MatlabR2010a software. ANN software serves as an initial tool for identifying the optimum network architecture for subsequent, in-depth inspection. During this step, guiding rules (Alyuda Research Company, 2003; Maier and Dandy, 2000; Palani et al., 2008) indicated that the potential N_h lies in the range 3–32.Within this range, the optimum value of N_h was determined following the trial and error approach. The search results demonstrated that the optimum network architecture was 8-3-1 and that it was obtained with the 75%-15%-15% partitioning scheme. The model predictions of the WQI produced by this network had a significant, positive, very high correlation coefficient with the experimental WQI values.

In consequence, the 150 water quality samples were divided into a training set made-up of 104 samples and cross-validation and testing subsets comprising 23 samples each. The network was trained using the feed forward back propagation algorithm. The WQI predictions of the 8-3-1 network trained using the BP algorithm had a significant, positive, very high correlation with the measured WQI values. This means that the ANN predictions of the WQI explain around 95.4% of the variations in the measured WQI values. This conclusion is reinforced by Figs. 3 and 4a,4b,4c. Fig. 3 compares the ANN-actual and the predicted WQI values for each single observation, while Fig. 4a,4b and 4c were a scatter plot of the model's WQI outputs versus the observed values, shows the training ,validation and testing results respectively. Both figures show that the overall agreement between the observed and simulated WQI values was satisfactory.

The ANN method for WQI calculation and forecasting offers some advantages over the traditional method. For the calculation of the WQI using this formula requires manual calculations whereby the raw data of eight water quality variables (pH, dissolved oxygen(DO), total dissolved solids(TDS), electrical conductivity(EC), total hardness, calcium (Ca) ions, magnesium(Mg)ions, and total alkalinity) have to be converted into sub-indices (Table 2,3) before the WQI can be calculated. The calculations are not performed on the parameters themselves but rather on their sub-indices whose values are obtained from the Table 2,3. To the contrary, the ANN approach utilized archived data to establish a model that can be used for direct calculation of the WQI from raw water quality variables without need for sub-indexing. The suggested ANN approach is therefore a more direct, rapid and convenient means of calculation of the WQI than the traditional method. Accordingly, this study accentuates that the ANN constitutes an effective tool for assessment of the water quality that simplifies the computation of the WQI and that saves substantial efforts and time by optimizing the calculation.

In other respects, we can still compare the outputs of the ANN model and those of the traditional method for WQI computation. The WQI values calculated using the traditional method were set as reference values for the ANN method. Actually, the traditional method is a statistical method where the WQI is calculated based on curve estimation models/equations. Both this method and the ANN approach are non-linear modeling techniques. However, the ANN approach to produce highly accurate estimates of the WQI is more successful that the WQI values calculated using the traditional method. And since the WQI calculated using the traditional method provided reference WQI values for the ANN model, i.e., it was set as the target for the corresponding neural network model, and then the performance of the ANN model can be evaluated by comparing its WQI outputs with those of the traditional method through correlation or regression analyses and/or graphical methods. The results (e.g., Figs. 3 and 4a,4b,4c) demonstrate that a reasonable approximation was made by the ANN model across the spectrum of the measured WQI values. The overall agreement between the measured and simulated WQI values was very satisfactory.

Conclusion

This study described the application of ANN to a prediction (or function approximation) problem entailing use of archival measurements on water quality variables of ground water for construction of a model capable of calculating and forecasting the WQI. It discussed common problems concomitant to design of ANN models, with example application on the groundwater at Batlagundu, and demonstrated effectiveness of the ANN approach in this particular field. The power of a neural solution in rendering satisfactory models based on a reduced set of predictors has also been illustrated. Eventually, a model based on the three-layer perceptron neural network was developed for computation of the WQI. The different potential models were trained and tested on monthly data of 8 water quality variables measured over a period of 24 months using a parallel, fully-connected, feed-forward network trained using the BP algorithm. Findings from this study emphasize that the ANN enables easy modeling of the WQI and allows identification of the comparative importance and contribution of input water quality variables to the model predictions. Accordingly, this study accentuates that the ANN constitutes an effective tool for assessment of the water quality that simplifies computation of the WQI and that saves substantial efforts and time by optimizing the calculation. Thereupon, the ANN approach presented in this article constitutes a useful, powerful alternative to traditional (or statistic) WQI calculation methods, especially those methods which involve lengthy computations and use of various sub-index formulae for each value or range of values of the constituent water quality variables. This approach can be commonly used and it can be applied equally successfully to any aquatic system worldwide. The study results should therefore encourage water quality monitoring authorities and water resource

ISSN: 2277-9655
Impact Factor: 1.852

managers to adopt ANN models as comprehensive and highly reliable alternatives to such WQI calculation methods. Therefore, empirical data analysis techniques such as the ANNs are recommended for analysis of long-term environmental monitoring records. The authors hope that this study and its outcomes provide a protocol for application of ANN models to WQI calculation.

Table 1 Descriptive statistics for the variables of the study area (All parameters in mg/l except pH & EC)

S.No	Parameters	Min	Max	Mean
1	pH	6.5	8.4	7.45
2	DO	4.8	8.4	6.6
3	EC	675	3137	1906
4	TDS	459	2133	2592
5	TA	195	403	299
6	TH	189	905	547
7	Ca	40	203	121.5
8	Mg	18	98	58

Table 2 Water Quality Factors their ICMR/CPHEEO Standards and AssignedUnit Weights

Water Quality Factors	ICMR/CPHEEO Standards (Vi)	Unit Weights(Wi)
pH	7.0-8.5**	0.322
TDS	<1500**	0.002
Hardness	<600**	0.005
Calcium	<75*	0.037
Magnesium	<50*	0.055
Total Alkalinity	<120*	0.023
Dissolved Oxygen	>5*	0.548
Electrical conductivity	<300*	0.009

*ICMR standards (1975) **CPHEEO Standards (1991)

Table 3 Rating Scale for Calculating WQI

Physico chemical Factors	Ranges				
pH	7.0-8.5	8.6-8.7 6.8-6.9	8.8-8.9 6.7-6.8	9.0-9.2 6.5-6.7	>9.2 <6.5
TDS	0-375	375.1-750	750.1-1125	1125.1-1500	>1500
Hardness	0-150	150.1-300	300.1-450	450.1-600	>600
Ca	0-20	20.1-40.0	40.1-60.0	60.1-75.0	>75
Mg	0-12.5	12.6-25.0	25.1-37.5	37.6-50	>50
Total Alkalinity	21-50	50.1-70 15.1-20	70.1-90 10.1-15	90.1-120 6-10	>120 <6
DO	>7.0	5.1-7.0	4.1-5.0	3.1-4.0	<3.0
EC	0-75	75.1-150	150.1-225	225.1-300	>300
V_r	100	80	60	40	0
Extent of Pollution	clean	Slight pollution	Moderate pollution	Excess pollution	Severe pollution

Table 4 WQI ranges as follows (Tiwari and Misra, 1985.)

Value of WQI	Quality of water
90-100	Excellent
70-90	Good
50-70	Medium
25-50	Bad
0-25	very bad

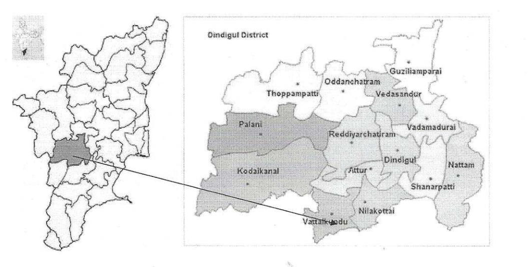

Fig.1 Map of the study area

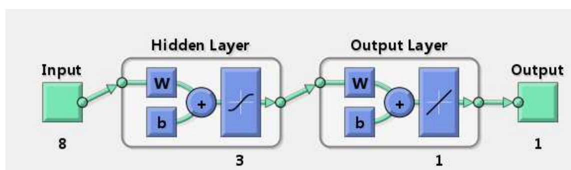

Fig.2 Optimal network architecture of the study

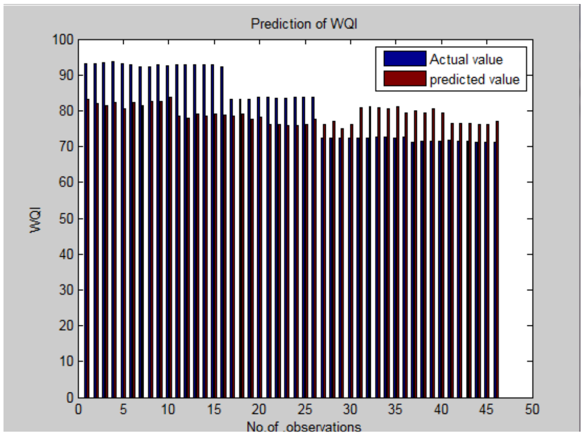

Fig.3 A graphical representation of the results of ANN mode

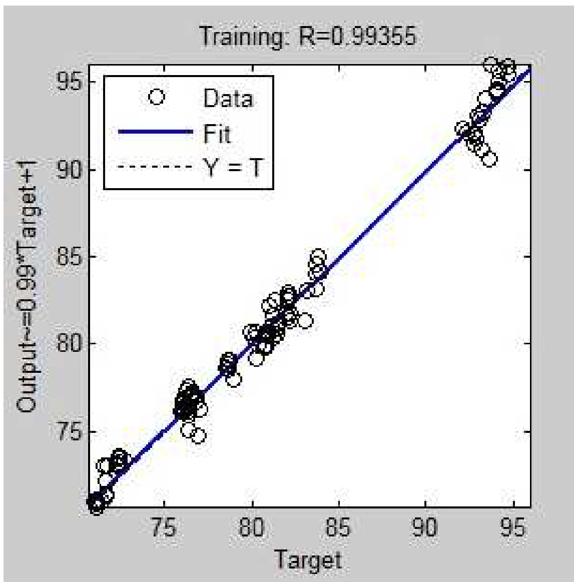

Fig.4a Scatter plot of Training data set for ANN model

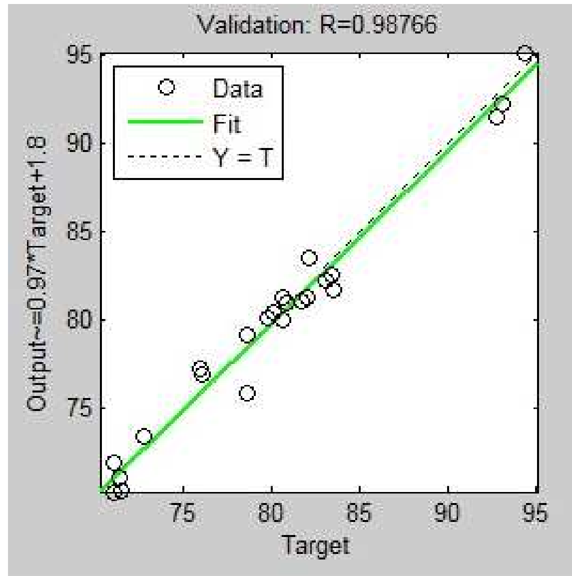

Fig.4b Scatter plot of validation data set for ANN model

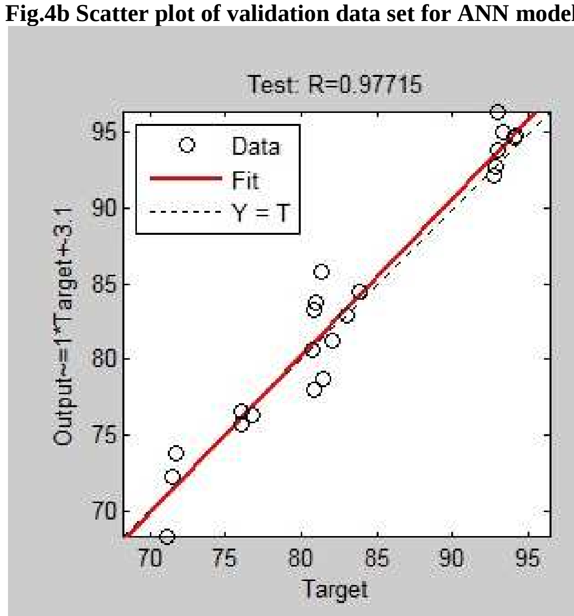

Fig.4c Scatter plot of Testing data set for ANN model

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