Pol. J. Environ. Stud. Vol. 24, No. 4 (2015), 1507-1515

Original Research

Artificial Neural Network Modeling of Dissolved Oxygen Concentrations in a Turkish Watershed

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Received: 13 September 2013
Accepted: 14 January 2014

Abstract

This paper presents the application of artificial neural networks (ANNs) and regression analysis (RA) for predicting dissolved oxygen concentrations (DO, mg/L) from water quality (WQ) indicators, namely stream water pH and temperature (t, ºC). For this purpose, three diverse models are used in our analysis, considering the functional relationship between *in situ*-measured WQ indicators and DO concentration. The WQ data are semimonthly obtained from nine monitoring sites in the Harsit Stream watershed in the Eastern Black Sea Basin of Turkey, from March 2009 to February 2010. As a result of model prediction, this study proposes a suitable ANN model, including two independent variables to efficiently predict DO concentration from WQ data, with the root mean square error of 0.9442 mg/L and mean absolute error of 0.6965 mg/L. The proposed model predicts the DO concentration better than the RA and the other two ANN models. The results may reduce the time and cost necessary to determine DO concentrations.

Keywords: artificial neural networks, dissolved oxygen concentration, Harsit stream watershed, pH, regression analysis, water temperature

Introduction

A sufficient supply of dissolved oxygen (DO) is vital for all higher aquatic life. The problems associated with low concentrations of DO in rivers have been recognized for over a century. The impacts of low DO concentrations or, at the extreme, anaerobic conditions in a normally well oxygenated river system, are an unbalanced ecosystem with fish mortality, odors, and other aesthetic nuisances [1].

Natural waters in equilibrium with the atmosphere typically contain DO concentrations in the range from 5 to 15 mg/L O_2 depending on water temperature, salinity, and altitude [2]. The DO concentration present in water reflects atmospheric dissolution, as well as autotrophic and heterotrophic processes that produce and consume oxygen, respectively. A fluctuation of DO near saturation, with diurnal variation due to temperature and metabolism, implies relatively healthy waters. By contrast, a marked depression of DO below saturation indicates a stream receiving untreated wastewater or an excessive amount of nutrients from non-point source pollution [3, 4].

Analysis of DO is extremely important in determining water quality. It provides information on the biological and biochemical reactions occurring in a water body, and is, therefore, an important indicator of stream metabolism [5]. *In situ* measurements of this parameter can be used as a primary indicator of water quality, and regulatory agencies recommend a minimum DO requirement

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for maintenance of fish populations, e.g. DO≥6 mg/L measured over at least one diurnal cycle [6]. For decades, DO concentrations have been used as a primary indication of water quality standards in aquatic environments. Much research has been devoted to understanding DO dynamics in streams [4].

The temperature of water is a very important parameter because of its effect on chemical reactions and reaction rates, aquatic life, and the suitability of the water for beneficial uses. Increased temperature, for example, can cause a change in the species of fish that can exist in the receiving water body. In addition, oxygen is less soluble in warm water than in cold water. The increase in the rate of biochemical reactions that accompanies an increase in temperature, combined with the decrease in the quantity of oxygen present in surface waters, can often cause serious depletions in DO concentrations in the summer months [7]. Temperature decreases cause an increase in the saturation concentration of DO. Changes in the saturation concentration affect the DO deficit and ultimately the reaeration driving force [8, 9].

Artificial neural networks (ANNs) are able to detect relationships in multi-dimensional data and organize this dispersed information into a nonlinear classification model [10, 11]. Recently, the neural networks approach has been applied to many branches of science. The approach is becoming a strong tool for providing hydraulic and environmental engineers with sufficient details for design purposes and management practices. The technique has a growing body of applications for river engineering and water resources [12-17]. ANN employment in DO estimation and prediction has been worked out for river water quality. Sengorur et al. examined the potential of ANN in estimating the DO concentration from limited data, namely nitrite nitrogen (NO_2^--N), nitrate nitrogen (NO_3^--N), biochemical oxygen demand (BOD), water discharge (Q), and temperature (t) measured monthly in the Melen River, Turkey, at 11 sampling points over a period of one year by employing feed-forward-type ANN for computing monthly values of DO concentration [18]. Basant et al. applied partial least squares regression and feed-forward back propagation ANN modeling methods to predict the DO and BOD levels using 11 input variables, namely pH, total alkalinity (T-Alk), total hardness (TH), total solids, chemical oxygen demand, ammonium nitrogen (NH_4^+-N), NO_3^--N, chloride (Cl^-), phosphate (PO_4^{3-}), potassium (K^+), and sodium (Na^+) measured monthly in the Gomti River, India, at eight different sites over a period of 10 years [19].

Ay and Kisi aimed to examine the accuracy of two different ANN techniques – the multilayer perceptron (MLP) and radial basis neural network – to estimate DO concentration using four input variables, namely pH, t, electrical conductivity (EC), and Q measured daily at the upstream and downstream of the Foundation Creek, El Paso County, Colorado, USA [20]. Wen et al. developed an ANN to simulate the DO concentrations using eight input variables, namely NH_4^+-N, calcium (Ca^{2+}), Cl^-, EC, NO_3^--N, pH, T-Alk, and TH measured monthly in the Heihe River, Northwestern China, at three water quality (WQ) monitoring stations over a period of six years [21]. Antanasijevic et al. created an ANN model using WQ indicators, namely pH, t, EC, and river flow measured monthly or semimonthly in the Danube River, north Serbia, at 17 WQ monitoring stations over a period of five years for prediction of DO concentrations [22].

The aim of this study is to research whether stream WQ indicators can produce a sufficient prediction of DO concentrations. A stream WQ monitoring study including 20 indicators was conducted on a semimonthly basis from March 2009 to February 2010 in the Harsit Stream watershed in the Eastern Black Sea Basin of Turkey. Of these indicators, by factor analysis, only two – namely pH and t – were selected as model input vectors.

Artificial Neural Network Approach

ANNs are human attempts to simulate and understand what goes on in the nervous system, with the hope of capturing some of the power of these biological systems. ANNs are inspired by biological systems with a large number of neurons that collectively perform tasks that even the largest computers have not been able to match.

The function of artificial neurons is similar to that of real neurons; they are able to communicate by sending signals to each other over a large number of biased or weighted connections. Each of these neurons has an associated transfer function that describes how the weighted sum of its input is converted to an output (Fig. 1).

Different types of ANNs have evolved based on neuron arrangement, their connections, and training paradigm used. Among the various types of ANNs, the MLP trained with back propagation algorithm has proven to be most useful in engineering applications. Back propagation is a systematic method for training MLP.

The MLP network comprises an input layer, an output layer, and a number of hidden layers (Fig. 2). The presence of hidden layers allows the network to present and compute more complicated associations between patterns. Basic methodology of ANNs consists of three processes: network training, testing, and implementations.

The connection weights of the ANN are adjusted through the training process, while training effect is referred to as supervised learning. The training of ANNs usually involves modifying connection weights by means of learning rule. The learning process is done by giving

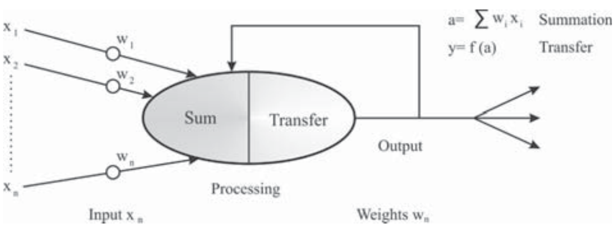

Fig. 1. Artificial neuron.

weights and biases computed from set training data or by adjusting weights according to a certain condition. Then, other testing data are used to check the generalization. The purpose of the bias input of a back propagation network is to stabilize the origin of activation function for providing better learning [23]. The initial weights and biases are commonly assigned randomly. As input data are passed through hidden layers, sigmoidal activation function is generally used. The data are uniformly selected during the training process. A specific pass is completed when all data sets have been processed. Generally, several passes are required to attain a desired level of estimation accuracy. Training actually means for each input pattern, and then compares it with the correct output. The total error based on the squared difference between predicted and actual output is computed for the whole training set. The adjustment of the weight corrections has been carried out using the standard error back propagation algorithm minimizing the total error (E) with the gradient decent method [24, 25].

Weight update formula in the back propagation algorithm is given as follows:

$$w_{j_{(L-1)}}h_L(t+1) = w_{j_{(L-1)}}h_L(t) + \alpha\delta^k_{h_L}x^k_{j(L-1)} + \eta\left[w_{j_{(L-1)}}h_L(t) - w_{j_{(L-1)}}h_L(t-1)\right] \quad (1)$$

…where α, η, L, and x^k are the learning rate, momentum parameter, layer number, and output vector, respectively.

The total sum squared error (TSSE) is calculated as follows:

$$\mathrm{TSSE} = \frac{1}{2}\sum_{i_0=1}^{N}\left(y^k_{i_0} - x^k_i\right)^2 \quad (2)$$

… where y^k is a desired output vector [26].

The foregoing algorithm used in this study updates the weights after an epoch is presented. (Epoch is one cycle through the entire set of training patterns.)

The Study Area

There are 26 hydrological basins in Turkey. With a recharge area of 24,077 km^2, the Eastern Black Sea Basin is one of the most important in Turkey, and is a major part of the Caucasus Ecological Region, together with the Coruh and Aras Basins. The Eastern Black Sea Basin consists of sub-watersheds such as Melet, Pazar, Karadere, Firtina, and Harsit streams, of which Harsit is the largest. The length of the main branch of the Harsit is 143 km; the catchment area is 3,280 km^2 [27-29].

The Harsit is formed by small streams that originate from the Vauk Mountains in eastern Gumushane Province. After it is formed, the Harsit passes through the settlements of Tekke, Gumushane, Torul, Ozkurtun, Kurtun, and Dogankent before emptying into the Black Sea at the city of Tirebolu [27-29].

The stream WQ monitoring studies were conducted every 15 days from March 2009 to February 2010 at 10 longitudinal stations from the upstream (H1) to the downstream (H10) in the Harsit watershed (Fig. 3), and their spatial information is given in Table 1.

Experimental Procedures

In situ DO, pH, and t measurements

The stream DO concentration (mg/L), pH, and t (ºC) were measured with a portable field meter (Horiba U-10). Moreover, these measurements were verified by another portable field meter (HQ40d).

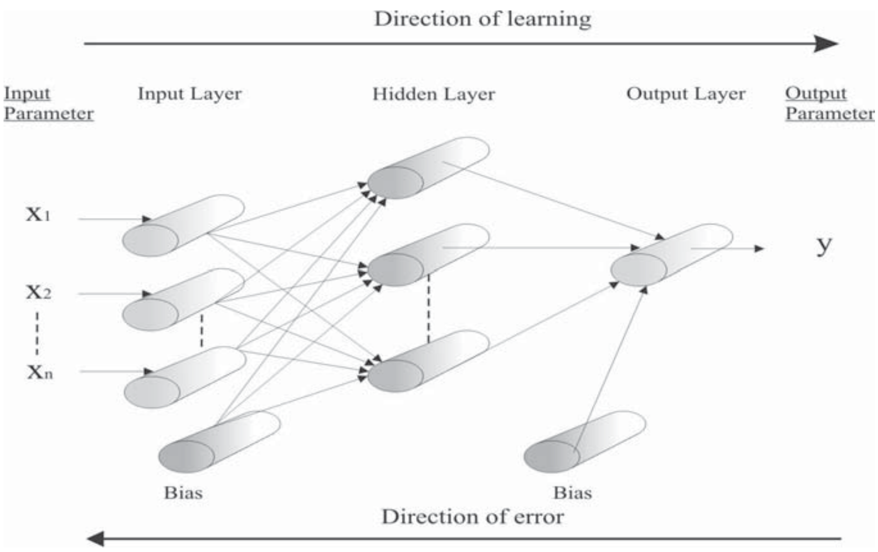

Fig. 2. Architecture of back propagation network model.

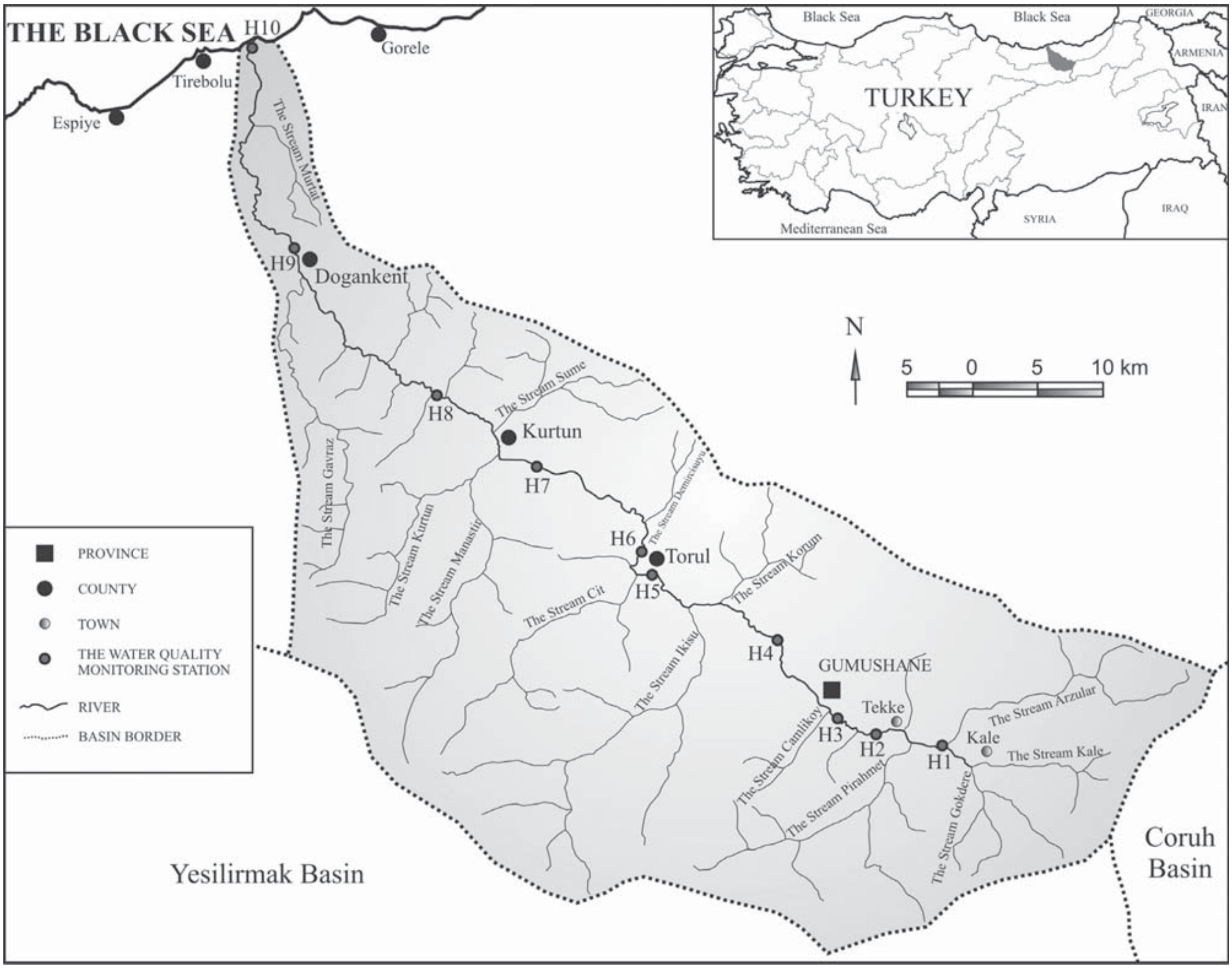

Fig. 3. The Harsit watershed and the locations of water quality monitoring stations.

Table 1. Location of the water quality monitoring stations in Harsit watershed.

Stations	Coordinates	Altitude (m)	Km of the course
H1	40º 24’ 07.4” N – 39º 38’ 29.3” E	1,274	0.0
H2	40º 24’ 54.0” N – 39º 34’ 37.6” E	1,234	6.5
H3	40º 25’ 23.6” N – 39º 31’ 37.7” E	1,190	12.5
H4	40º 29’ 36.6” N – 39º 27’ 30.4” E	1,100	24.0
H5	40º 32’ 55.7” N – 39º 18’ 52.5” E	939	39.5
H6	40º 33’ 56.7” N – 39º 17’ 54.6” E	910	45.0
H7	40º 38’ 41.1” N – 39º 11’ 01.4” E	642	67.5
H8	40º 42’ 18.5” N – 39º 04’ 11.8” E	497	84.0
H9	40º 49’ 18.6” N – 38º 54’ 42.5” E	154	107.0
H10	41º 00’ 16.1” N – 38º 50’ 59.7” E	4	137.0

Table 2. Regression coefficients and R^2 value for regression analysis.

Model no	c	b_1	b_2	b_3	R^2
1	10.277750	-0.767324	0.000000	0.012921	0.275
2	9.729723	0.560693	-0.067181	0.001921	0.324
3	2.073186	1.178817	-0.076864	–	0.388

Prediction of DO Concentration

Regression Model

Multiple linear and nonlinear (exponential, power, logarithmic, inverse, joint, growth, and S functions) regression analyses were performed. Three models producing satisfactory results are presented as follows:

$$\text{Model 1: } \textit{DO concentration} = c + b_1\,pH + b_2\,pH^2 + b_3\,pH^3 \quad (3)$$

$$\text{Model 2: } \textit{DO concentration} = c + b_1\,t + b_2\,t^2 + b_3\,t^3 \quad (4)$$

$$\text{Model 3: } \textit{DO concentration} = c + b_1\,pH + b_2\,t \quad (5)$$

In these equations, b_1, b_2, b_3, and c are the regression coefficients, estimated by the least squares method for all of the models. The R^2 values for the models are given in Table 2.

ANN Model

The main objective of this section is to develop an ANN model that predicts the DO concentration from given pH and T data. When designing an ANN, it is important to choose the proper network size. If the network is too small, it may not have enough free parameters to represent the data adequately. If the network is too big, it can either fail to classify the data as meaningful categories or reject new patterns as too dissimilar from the training set. In general, finding a suitable network structure is a matter of trial and error, although an educated guess can be made by comparing the size of the training data set to the number of free parameters in the network. As shown in Fig. 2, a three-layer, feed-forward network is selected for this study. Each layer is fully connected to the next, but no connections exist between neurons in the same layer. The first and third layers contain the input and output variables, respectively. Three different models were used to train the neural network (Fig. 4). The DO concentration is the output variable for all models. The order of variables in the input layers is pH and t.

The stream WQ data from the eighth station (H8), where the stream DO concentration was unusually positive correlated with stream t were excluded, and the rest of data set 216 was divided into 162 training (75%), 36 testing, and 18 validation patterns. Input values for the testing, training, and validation data are shown in Table 3.

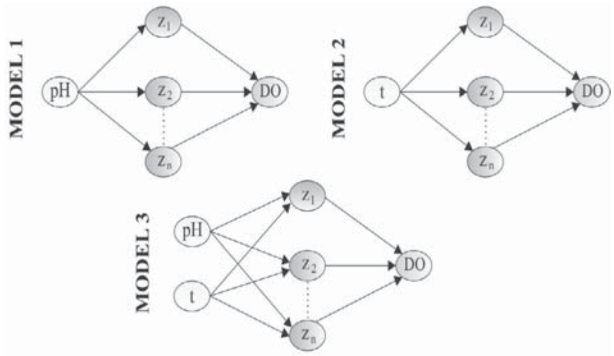

Fig. 4. ANN architectures used for the prediction of the DO concentration.

Before the training of the network, the data are normalized to range [0.1, 0.9] since the sigmoid activation function is used.

The selected network size represents a compromise between generalization and convergence. Convergence is the capacity of the network to learn the patterns in the training set, and generalization is its capacity to respond correctly to new patterns. One hidden layer is sufficient for most applications [30]. Since determining the number of nodes in the hidden layer is not an exact science, several networks with different numbers of hidden nodes are tested. The parameters of the optimum ANN structures are given in Table 4. To begin the training process, all of the training patterns are introduced to a network initialized with random weights. All the computations were conducted using MATLAB software (The MathWorks, Inc., Natwick, MA).

In this study, the weights are initialized into random values between -0.5 and +0.5, according to commonly accepted procedure. The factors α and η in Eq. (1) also influence the convergence. The learning rate (α) is the constant of proportionality for the generalized back propagation rule. The larger its value, the greater the changes in the weights. The momentum term (η) is used to prevent the network from oscillating around a local minimum in the parameter space. Several combinations of α and η are tested in order to find a neural network with good convergence (Table 4).

Memorization (over training) is a fundamental problem encountered in training of ANN. To prevent this, the training is terminated when the network begins

Table 3. Semimonthly water quality data set used in the ANN models.

The stations	Water quality monitoring period: March 2009–February 2010																							
	Spring						Summer						Autumn						Winter					
H1	●	●	●	▲	●	●	●	●	▲	●	●	■	●	●	▲	●	●	●	●	■	●	●	●	▲
H2	●	●	▲	●	●	■	●	●	●	▲	●	●	■	●	●	▲	●	●	●	●	●	▲	●	●
H3	●	●	●	●	●	▲	●	▲	●	●	■	●	●	▲	●	●	●	●	▲	●	●	●	●	■
H4	●	▲	●	●	■	●	●	●	●	●	●	▲	●	●	●	■	●	▲	●	●	●	▲	●	●
H5	●	●	●	●	▲	●	●	■	●	●	▲	●	●	■	●	●	▲	●	●	●	▲	●	●	●
H6	▲	●	■	●	●	●	▲	●	●	●	●	●	▲	●	●	●	■	●	●	●	●	●	▲	●
H7	●	■	●	▲	●	●	●	●	●	▲	●	●	●	●	▲	●	●	●	●	▲	●	■	●	●
H8	–																							
H9	●	▲	●	■	●	●	●	●	●	●	▲	●	●	●	●	●	●	▲	●	▲	●	●	■	●
H10	●	●	●	●	●	▲	●	▲	●	■	●	●	●	▲	●	●	●	●	■	●	●	●	●	▲
● = training set, ▲ = testing set, ■ = validation set																								

to memorize by using the cross-validation patterns [31]. In this situation, training set error continues to decrease, although testing set error does not change. The performance of a network may be enhanced by increasing the number of training samples, the length of training (number of epochs), or the number of hidden layer nodes. Choosing different values for α and η may also change the performance of a network. However, all of these methods increase the computation time required to train the network. It is very important to strike a balance between performance and training time. Table 5 shows the ANN structures that yield the best results.

The root mean square error (RMSE) and the mean absolute error (MAE) were used to provide an indication of goodness of fit between the monitored and modeled values.

The RMSE is calculated as follows:

$$\mathrm{RMSE} = \left[\frac{1}{\mathrm{N}}\sum_{\mathrm{i}=1}^{\mathrm{N}}(\mathrm{P_i} - \mathrm{O_i})^2\right]^{\frac{1}{2}} \tag{6}$$

The MAE is calculated as follows:

$$\mathrm{MAE} = \frac{1}{\mathrm{N}}\sum_{\mathrm{i}=1}^{\mathrm{N}}|(\mathrm{P_i} - \mathrm{O_i})| \tag{7}$$

…where N is the number of observations, O_i is the i^{th} observed value, and P_i is the i^{th} predicted value.

Results and Discussion

When the ANN analysis was performed with models 1, 2, and 3, the minimum error in the testing set was obtained as 0.371 for the third model (α = 1.00 and η = 0.10) (Table 5). The errors may be reduced if the stopping criterion, the epoch number, is increased. Besides, conjugate gradient or scaled conjugate gradient methods may be used to reduce maximum relative error instead of generalized delta rule in learning. Also, different network structures with one or more hidden layers or nodes with different learning rates and momentum terms may produce less error.

Table 4. Parameters used for different ANN structures.

Number of hidden layer unit	Learning rate (α)	Momentum (η)
3, 5, 7, 10	0.10	0.10
	0.25	0.25
	0.50	0.50
	0.75	0.75
	1.00	1.00

Table 5. Characteristics of ANNs yielding the best results.

Model no	Number of hidden layer unit	α	η	Epoch	Training error[a]	Testing error[a]
1	7	0.50	1.00	9301	1.65635	0.53629
2	3	0.25	0.50	20000	1.57270	0.40900
3	2	1.00	0.10	14625	1.16183	0.37107

[a] Error values are calculated from Eq. 2.

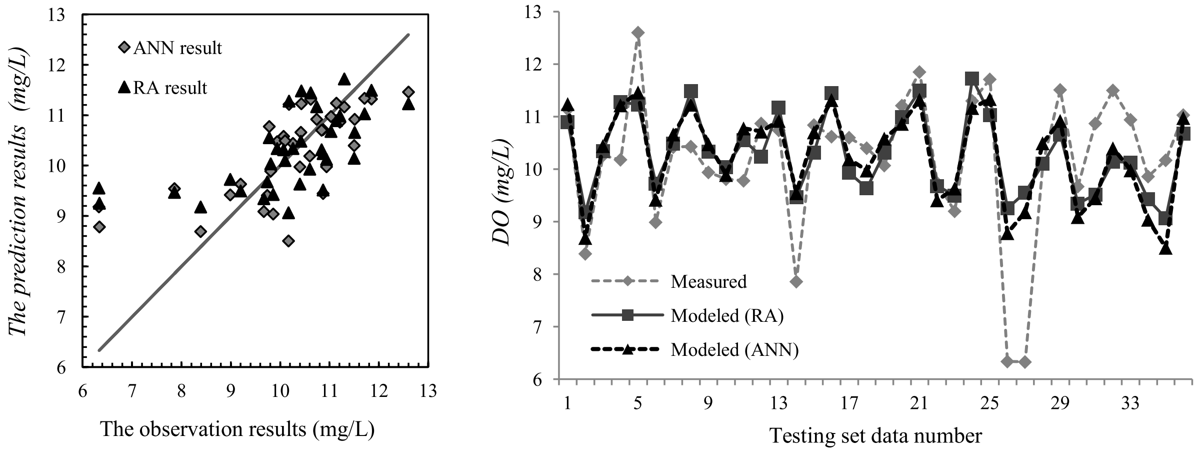

Fig. 5. The comparison of the observed DO concentrations with the predicted ones for testing set.

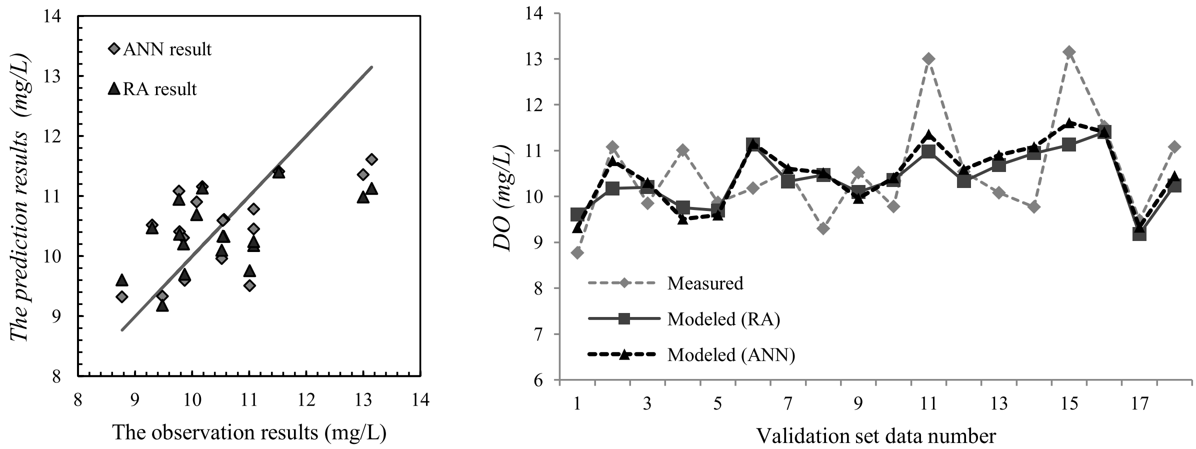

Fig. 6. The comparison of the observed DO concentrations with the predicted ones for validation set.

Figs. 5 and 6 display the performances of the ANN and regression analyses for the testing and validation data, and the accuracy of the ANN approach for the best-fitting model (the third model). Each quad sign stands for testing and validation vectors in both figures. Also, the results obtained from RA for the same values are shown with multiple signs in the same figures. The nearer the points gather around the diagonal, the better the learning results. The RMSE and MAE of the points on the diagonal are zero. While the RMSE and MAE values obtained from the testing set for the ANNs in the third model are 0.944 and 0.697 mg/L, these values for the RA in the same model are 1.027 and 0.759 mg/L, respectively. Similarly, the RMSE and MAE for the validation set in the ANNs in the third model are 0.623 and 0.710 mg/L, and the same values for the RA are 0.967 and 0.787 mg/L, respectively (Table 6).

Conclusions

The preceding sections have dealt with the development of regression analysis (RA) and artificial neural network (ANN) models to predict dissolved oxygen concentration (DO, mg/L) using water quality (WQ) indicators, namely

Table 6. The error values for each method in terms of mg/L.

Model no	RMSE for testing		MAE for testing		RMSE for validation		MAE for validation	
	ANNs	RA	ANNs	RA	ANNs	RA	ANNs	RA
1	1.13511	1.13390	0.82643	0.82739	0.717751	1.00233	0.83683	0.82637
2	0.99166	0.99201	0.69022	0.69327	0.725334	1.04627	0.78599	0.79651
3	0.94415	1.02703	0.69652	0.75859	0.623321	0.96730	0.70961	0.78700

water pH and temperature (t, ºC) in the Harsit watershed of northeastern Turkey. For this purpose, three different models are constructed, considering the variety of independent variables. The following conclusions are drawn:

– This paper proposes a suitable ANN model including two independent variables: pH and t. The model has a root mean square error of 0.9442 mg/L and a mean absolute error of 0.6965 mg/L.
– Among the RA models, the model considering t in the input vector can be suggested as a prediction tool for the DO concentration.
– The ANNs model provides satisfactory prediction of the DO concentration using a limited number of the WQ indicators. This may imply that the model can be a useful tool for the prediction of the DO concentration in Turkish streams and rivers. Therefore, the ANNs model may provide great convenience in water research and for environmental managers.

Acknowledgements

The authors would like to thank Prof. Dr. Hızır Önsoy, Prof. Dr. Mehmet Tüfekçi, Prof. Dr. Talat Şükrü Özşahin, Assoc. Prof. Dr. Volkan Numan Bulut, Asst. Prof. Dr. Mustafa Durmaz, Asst. Prof. Dr. Tayfun Dede, Aydın Bayrak, and Yüksel Hardal for their valuable support. This paper is dedicated to the memory of the late Assoc. Prof. Dr. Murat İhsan Kömürcü, who supported this work tremendously, serving as research assistant, Ass. Prof. Dr., and Assoc. Prof. Dr. at the Hydraulic Laboratory, Department of Civil Engineering, Faculty of Engineering, Karadeniz Technical University until his death in 2013.

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