



Application of an Artificial Neural Network Model for Estimating Water Quality Parameters in the Karun River, Iran

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Abstract

Population growth and increasing agricultural and industrial activities result in reducing water quality, climate change, and changed the rainfall pattern as well as the hydrological cycle. In the present study, artificial neural networks (ANN) applied deduced and expand models to predict the monthly values of dissolved oxygen (DO), and electrical conductivity (EC) in the Karun River at stations positioned at Ahwaz and Gotvand sites in Iran. To analyze the water quality, the monthly data of four main parameters and discharge between 1998 and 2010 were selected. The correlation coefficient, root mean square error, and mean absolute error as statistical criteria were utilized for evaluating the model performance. Finally, the potential of ANN on simulating relevancy between water quality parameters is examined. Results indicated the neural networks can discern the pattern of water quality parameters to offer an appropriate prediction of changes in water quality data of the Karun River.

Keywords: Artificial Neural Networks, Predicting, Water Quality Index, Khuzestan province

1 Introduction

Water is a crucial resource that human needs for the existence life [1], and the water consumed for drinking, especially in third world countries, irrigation, industrial, recreation, tourism, etc. that is mainly provided with rivers [2-4]; hence, its quality should be at least in the acceptable standard range, and preserving of surface water is of great importance as well as short and long-term planning and managing of the resources to optimize their performance [5]. There are a variety of models and methods for solving water quality management issues due to the new sophisticated modeling tools, and select the suitable one depends on modeling studies and considered variables [6-7]. Selecting the proper variables are quite complicated since the chosen variables to be sampled mainly is influenced by the objective and economics of monitoring [8]. By choosing the suitable model and method, the number of variables can be reduced provided that a significant correlation is detected [9]. The water shortage, increasing temperature, decreasing precipitation, overpopulation, growing demand for water, energy crisis, and increasing concentration of pollutants in water resources are growing worldwide issues that challenging the sustainable expansion in the macrocosm [10-12]. Therefore, the basic problem in the management of aquatic environments is the river water quality properties and procedures evaluation [13-14]. There are many detrimental points in the river water quality properties simulation like cost-effective simulation, saving time, eliminate the requirements for laboratory and measuring equipment, removing the laboratory errors,

regeneration missed data, calibrating measurement equipment, etc. [15]. To evaluate the river water quality, different parameters such as dissolved oxygen (DO), which is a significant quality index of water resources, chemical oxygen demand (COD), Potential Hydrogen (pH), temperature, and electrical conductivity (EC) can be considered [16]. However, traditional mathematical methods make it hard to measure DO concentration owing to the influences of various parameters on different rivers' water [17].

Over the last decades, many different applications of ANN have been used for predicting and water quality, and determine its qualitative tests using independent variables [18-22]. Many studies have been carried out using ANN for modeling water quality in evaluating DO concentration, groundwater calculations, and fluctuations, predict groundwater depth, predict turbidity of rivers, etc. [23-28]. Vasanthi and Kumar studied the application of ANN to predict the seven water quality index parameters in the Parakai lake at four monitoring stations from December 2016 to March 2018. The results showed that the ANN model foretells the water quality indicators more precisely rather than the multiple linear regression (MLR) [22,29]. Salami et al. evaluated the rate of DO and temperature of surface water in a case in California, and the results represented that the value of DO, on an average basis, the changing rate in the region of study is -0.138 mg/l.year, and the average rate of temperature is +0.02°C/y. [14]. Although ANN has a strong theoretical potential, its application has been subjected to some challenges. The generalization of an ANN is dependent upon the network

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topology and chosen of prominent network parameters, comprising the transition and error function, learning rate, and momentum [30]. A time-effective approach which is a trial and error approach is usually utilized for optimizing the ANN model. For selecting the network architecture there are two kinds of automated techniques, namely pruning and constructive algorithms [31].

Over the past two decades, the performance and application of ANN have been successfully developed in various fields, especially water resources [32-37]. One of the capabilities of the multilayer neural network is to estimate a measurable performance with respect to input and output vectors by selecting the appropriate set of connection weights and transmission functions. [38]. Consequently, ANNs can model the environmental systems regardless of initial consideration of algebraic relationships among variables which had resulted in its application in water resources performances [39-41].

This study used an artificial neural network model developed to anticipate (DO) and (EC) based on monthly measured water quality data at the Gotvand and Ahwaz stations of Karun river, which location is shown in Fig. 1. The basis selection of input variables for ANN is statistical correlation analysis and the availability of the field data. In this paper, we aim to specify the DO concentrations as well as EC in the Karun river using continuous monthly measurements of selected variables such as temperature, discharge, and pH. The possibility of training ANN model correlating for the initial water quality variable as an independent variable (temperature,

discharge, and pH) along with secondary attribute as dependent (DO and EC) variable were investigated.

2 Materials and Methods

2.1 Water Quality Data and Study Region

Khuzestan Province is located in the southwestern of Iran which occupies an area of 64,236 square kilometers with geographical attributes from 47 degrees, 41 minutes to 50 degrees, 39 minutes the east of the meridian Greenwich and 29 degrees, 58 minutes to 33 degrees, 4 minutes of the north latitude from the equator. The geographical and hydrological conditions in the province in terms of having the highest share in the country's freshwater. It is evident with optimal quality and quantity of agricultural production will be faced with serious problems. The Ahwaz station is between 48 degrees, 41 minutes of the east longitude, and 32 degrees, 31 minutes of the north latitude. The height of Khuzestan is 16 meters above the sea, and it had an average discharge of 764 ft³/s during the period from 1998 to 2010. The geographical attributes of Gotvand station are between 48 degrees, 49 minutes of the east longitude, and 32 degrees, 14 minutes of the north latitude. Gotvand stations are 71 meters above sea level, and their average discharge was 441.2 ft³/s between 1998 and 2010 [35]. The water quality attributes in the ANN model territory considered from 1998 to 2010 in the Ahwaz and Gotvand stations are represented in Table 1 and 2, respectively.

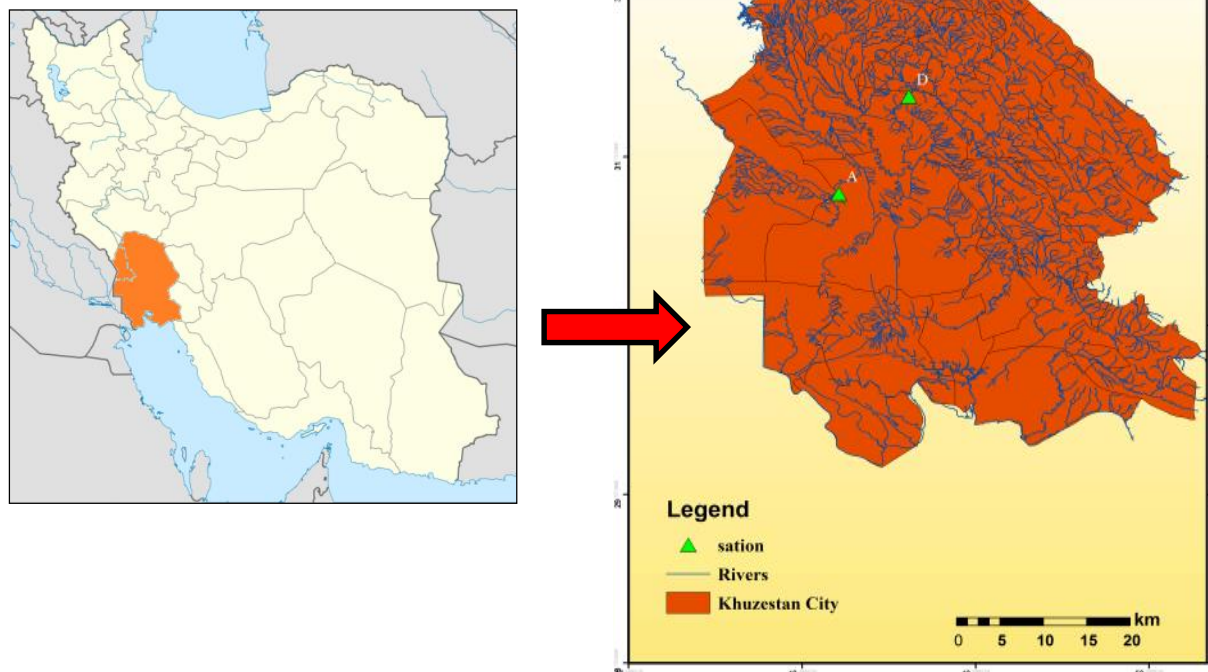


Figure 1: The position of the Karun River, Iran

Table 1: Water quality properties between 1998 and 2010 in the Ahwaz station

Parameter	Unit	Minimum	Maximum	Average	SD
Temperature	°C	12	31	20	5.3
pH	-	7.3	8.6	8	0.27
Discharge	m ³ /sec	147.8	3473	764.3	727.2
DO	Mg/l	3.18	9.12	6.89	1.06
EC	µs/cm	763	3045	1648	543

Table 2: Water quality properties between 1998 and 2010 in the Gotwand station

Parameter	Unit	Minimum	Maximum	Average	SD
Temperature	°C	8	50	19.6	5
pH	-	7.5	8.6	8.07	0.22
Discharge	m ³ /sec	1341.9	2224.3	441.2	507.4
DO	Mg/l	5.3	10.4	7.7	0.99
EC	µs/cm	515	2416	970.4	364.3

2.2 Basic Principles of ANN

In the present study, the concentration of DO and EC as the water quality parameters was estimated with an empirical neural network algorithm. It is difficult to simulate the DO, which is a substantial water quality index, by prevalent mathematical methods because various elements affect different water sources [8]. Moreover, the parameter EC is another important factor that is used as a general water quality indicator due to the dilution impact of streamflow. Indicators could be used for river contamination testing, or other resources of pollution have entered a stream. With regards to EC, the ANN model was extended for simulating and predicting the EC at Karun river, ANN introduced in 1943 by McCulloch and Pitts, and it works noticeably efficient when there is an extended number of variables or data compared to the conventional methods that the relationships between variables are vaguely understood [37].

ANN, which is a computational system, is made up of countless interconnected sets of simple data processing components, similar to a neuron, called a unit. Neurons collect input from multiple, single sources and provide an output based on predetermined nonlinear functions. ANN models, which are flexible and widely used in relation to water resources instead of classical methods, are built by connecting a large number of neurons in a known configuration. ANN is a logical programming system created by imitating the processes of the human brain. The training method is created between neurons and is done using known inputs and outputs and presents them in a transparent way to ANN [38]. The salient advantage of ANN is its ability to simulate complex nonlinear relationships regardless of the nature of the relationships by default. From the previous data (X_{t-1} , X_{t-2} , ..., X_{t-p}) to the future value X_t , the ANN model does a nonlinear functional mapping such as equation No. 1.

$$X_t = f(X_{t-1}, X_{t-2}, \dots, X_{t-p}) + et \quad (1)$$

where X and f have a vector of all parameters and a function specified by the network structure and connection weight. Therefore, ANN is equivalent to a nonlinear autoregulation model, and training of this program is necessary to achieve the desired results. The most important feature of ANN is difficulty training by adjusting the weights assigned to the available information and then recalling it. ANN is a method for video and audio recognition, speech analysis, decision making, control, and the definition of complex models. This program

differs from different aspects of classical programming by considering the working principles of the human brain. In this technique, the neurophysiological work of the human brain is performed by artificial neurons in a computer. Neurons are the structural elements of the human brain and perform operations in milliseconds. Among the several existing learning algorithms, republishing has been the most popular and widespread learning algorithm of all neural network paradigms [39-40]. In most ANN programs, the feedback error amplification neural network is the most well-known and widely used ANN architecture and is also used in this study. There are three basic levels of data processing: input layer, hidden layer, and output layer, each of which contains processing units called neural network nodes.

An example of ANN is shown in Figure 2.

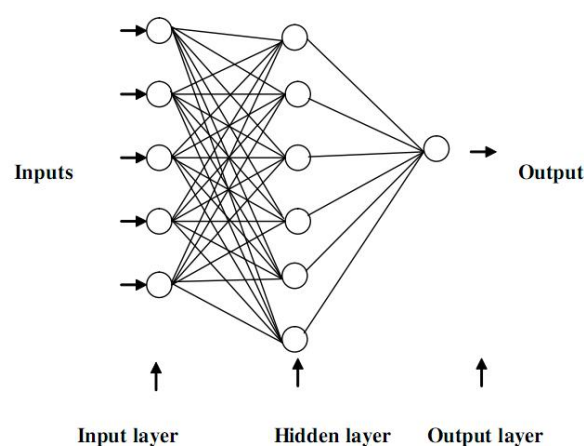


Figure 2: Structure of a multi-layer (input, hidden, and output layer) feed-forward ANN model

2.3. Back Propagation Neural Networks

Learning Algorithm: One of the typical used learning algorithms is the backpropagation (BP) [41]. The mentioned algorithm is in accordance with the generalized delta suggested by Rumelhart et al. 1986, was utilized to train the ANN in this paper. A group of inputs and outputs are chosen from training set in this algorithm, and the output is calculated based on inputs by the networks. The output-layer error is the difference between the actual output and this output. The error is back-

propagated through the network, the weights also are normally adjusted.

The objective function is to minimize the mean square error over the training sample. The back-propagation of the error gradient is used. This training algorithm is a method that causes the distribution of error to reach the optimal point or minimum error. At first, the information passes through the network in a straight direction. Then, an output is anticipated, the BP algorithm redistributes the error accompanied with this output back through the model, and weights are well-adjusted. Minimizing the error is obtained through various repetitions. After the training is fulfilled, the ANN performance is validated. Based on the result, the ANN has to be retained or it can be accomplished for its goal-oriented usage. In this paper, before the training of the network input and output variables were normalized in the range of 0.1 to 0.9 as follows:

$$x_i = 0.8 \frac{(x - x_{\min})}{(x_{\max} - x_{\min})} + 0.1 \quad (2)$$

where x is the measured value for the parameter, $x_{\min}$ and $x_{\max}$ are the minima and maximum values in the database for the parameter, respectively [42].

Training: To determine the ANN weights, the training procedure should be performed which is similar to the calibration of a mathematical model, so the ANN is trained using a training set of input data as well as unknown outputs. The weights should be initialized according to some previous experience, or with a set of random values to start the training process, aiming to specify a set of weights that can minimize the error function [39-41]. As training proceeds, the weights are systematically updated according to a training rule. Several training examples should be presented to the network, so the training procedure is completed when the difference between the measured and estimated value is less than a specified value, and the ANN is considered trained in this stage. Consequently, the ANN is trained to produce estimated outputs vector when Y_{9n0} presented with an input pattern X_{9n0} , and the function in the n^{th} input exemplar, $E(n)$ is as follow:

$$E(n) = \frac{1}{2} (\bar{Y}(n) - Y(n))^2 \quad (3)$$

where $\bar{Y}(n)$ is the estimated state of the output unit in response to the n^{th} input exemplar, and $Y(n)$ is the desired state of the output unit. After the $(n+1)^{\text{th}}$ input exemplar is presented, the weight is generally updated by:

$$\Delta w_{ji}(n+1) = -\eta \frac{\partial E}{\partial w_{ji}} - \xi \Delta w_{ji}(n) \quad (4)$$

where η stands for the learning rate, which for practical purposes is chosen as high as possible regardless of causing the oscillation of the convergence of the network, ξ is a constant (momentum term) that determines the effect of past weight changes on the current weight change.

Performance: By comparing the predictions of the model trained on the training set to the measured values in the overfitting test set, the model can be evaluated, and the values calibration is done using systematically adjusting various model parameters. Moreover, there are some features to evaluate the performance of the models namely, the root means square error (RMSE), the mean absolute error (MAE), and the correlation coefficient R that are represented in Eq. 5-7, respectively.

$$RMSE = \left[\sum_{p=1}^N \frac{(d_p - x_p)^2}{N} \right]^{\frac{1}{2}} \quad (5)$$

$$MAE = \frac{1}{N} \sum_{p=1}^N |d_p - x_p| \quad (6)$$

$$r = \frac{N \sum_{p=1}^N d_p x_p - (\sum_{p=1}^N d_p)(\sum_{p=1}^N x_p)}{\sqrt{[N \sum_{p=1}^N d_p^2 - (\sum_{p=1}^N d_p)^2] \times [N \sum_{p=1}^N x_p^2 - (\sum_{p=1}^N x_p)^2]}} \quad (7)$$

where d_p is the desired (target) value, x_p the ANN output for the p^{th} pattern, and N the total number of patterns. To present the visual comparison between observed and prediction values, Scatter and time series plots are used. The values of R^2 from zero indicate that the average observed as a model is a good predictor, and the values of R^2 one and negative indicate that the observed average is appropriate and a better predictor of the model, respectively. Based on the sensitivity of water quality parameters and the mismatch between the predicted and measured water quality variables, it is behind the expert decision that, is the predictability of the ANN model accurate enough to make important decisions about data usage?

3 Result and Discussion

To identify the maximum amount of the hidden layers and transfer function, several ANN models were created and examined. Monthly data portioned training (almost 70 percentage of the whole) and data sets have been used for neural network structure. Two water quality parameters have been chosen to be used as output (DO, EC) for the ANN models structure and three other water quality parameters (temperature and pH) and discharge (Q) have been considered to be used as input. In this survey, we have tried to figure out and measure the subsequent compositions of the input data of flow: pH, Temperature, and Discharge. There was 1 neuron for DO or EC in the input layer. We have selected a configuration for both compositions which are giving us the least RMSE for those compositions of DO models with pH inputs that have been demonstrated in diagram 2 (a,b). Hence it is obvious that other ANN models couldn't perform better than Temperature and Discharge (input composition 3). Different MLP networks have been and examined for the input composition3. BPA or Back Propagation Algorithm has been used to regulate the process and the flow of learning it also has been used to modify and rectify the networking momentum and weight decay. Diagram3 (a, b) is illustrating the outcomes of different MLP and their errors for DO. These are the outcomes that are already derived from the rows of unlearned data. From the subsequent equations, we have calculated MAPE or Mean Absolute Percentage Error for each model. If the favorable target value is d_p , x_p will be ANN output for the P^{th} patterns.

$$\text{Mean absolute percentage error (MAPE)} = \frac{1}{N} \sum_{i=1}^N \frac{|x_p - d_p|}{d_p} \quad (8)$$

The number of neurons in the hidden layer changed from 4 to 7 in this experiment. Since it is shown in diagram 3(a, b) outperforms other models with the use of some procedures the optimal EC model was created. Diagram 4 (a ,b) also is indicating the optional compositions with somehow better

prognosticated outcomes for both variables which were used as outputs. Diagram 2(a, b) is illustrating the connection and the relationship of the factor (r) RMSE and MAE valences. These values were calculated for the pedagogy and test data sets. The plot betwixt the measured and the calculated valences of DO (by ANN) in pedagogy and confirmation sets were shown in figure 4(a, b). Three nodes in the output layer five nodes in the hidden layer and a single node in the output layer were chosen as ANN and they've prepared an outstanding and suitable model for both data sets. Figure 2 (a, b) is indicating a precise template of conversion by evaluated and calculated DO condensation in the water of the river, RMSE and MAE valences indicate a suitable model fit for data sets.

Another correlated one with the main quality parameters of water due to the efficiency of streamflow is called EC. Hence it can be used as a popular and common water quality index (indicator). If Discharge or any other source of contamination enters the water stream (as an indicator) remarkable changes and alternation in conductivity will take place. For simulating and predicting the EC at Karun River Iran the ANN model has been developed. ANN Architecture Back Propagation (ABP) was used for two stations with a hidden layer and a hyperbolic-tangent transfer function, by both DO and EC. As it is explained before three nodes in input and four nodes in hidden layers and a single node in the output layer were selected. As an ANN they have produced a remarkable model for (the training and the examination) data sets.

Table 2(a): RMSE and Coefficient of correlation for ANN model-training and testing data in the Ahwaz station

ANN model input	Training Data DO (mg/lit)		Validation Data DO (mg/lit)	
	Correlation	RMSE	Correlation	RMSE
pH and Temperature	0.972	0.186	0.978	0.090
pH and Discharge	0.981	0.122	0.989	0.079
Temperature and Discharge	0.979	0.150	0.984	0.083
pH, Temperature and discharge	0.98	0.111	0.99	0.07

Table 2(b): RMSE and Coefficient of correlation for ANN model-training and testing data in the Gotvand station

ANN model input	Training Data EC (us/cm)		Validation Data EC (us/cm)	
	Correlation	RMSE	Correlation	RMSE
pH and Temperature	0.973	0.112	0.972	0.117
pH and Discharge	0.987	0.091	0.989	0.072
Temperature and Discharge	0.982	0.099	0.984	0.080
pH, Temperature and discharge	0.99	0.082	0.99	0.067

Table 3 (a): Different MLP results for DO in the Ahwaz station

MLP model number	1	2	3	4	5
Number of neurons in the first hidden layer	3	4	4	5	5
Number of neurons in second hidden layer	1	0	1	0	2
Relative error (MAPE)	0.0521	0.0470	0.0523	0.0429	0.0601

Table 3 (b): Different MLP results for DO in the Gotvand station

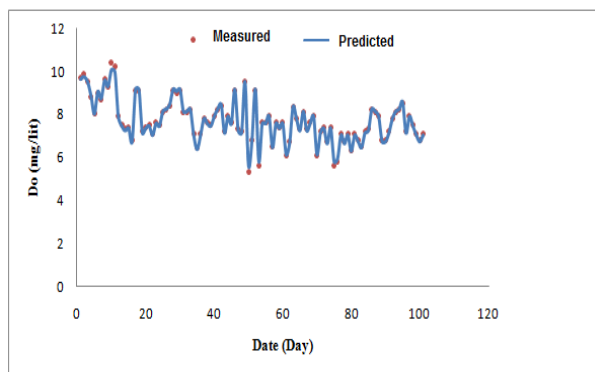
MLP model number	1	2	3	4	5
Number of neurons in first hidden layer	3	4	4	5	5
Number of neurons in second hidden layer	1	0	1	0	2
Relative error (MAPE)	0.0474	0.0463	0.0480	0.0471	0.0497

Table 4 (a): Results of ANN model parameters for calculating DO and EC in Karun river water (Ahvaz station)

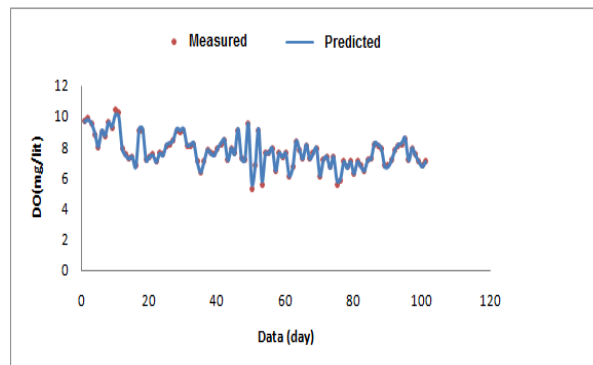
Model	ANN-Structure	Data set	RMSE	MAE	r
DO	3-5-1	Training	0.1	0.058	0.98
		Validation	0.07	0.039	0.99
EC	3-3-1	Training	55.2	37.98	0.97
		Validation	37.03	29.87	0.97

Table 4 (b): Results of ANN model parameters for calculating DO and EC in Karun river water (Gotvand station)

Model	ANN-Structure	Data set	RMSE	MAE	r
DO	3-4-1	Training	0.082	0.055	0.99
		Validation	0.067	0.055	0.99
EC	3-5-1	Training	35.2	24.7	0.97
		Validation	37.4	31.4	0.96

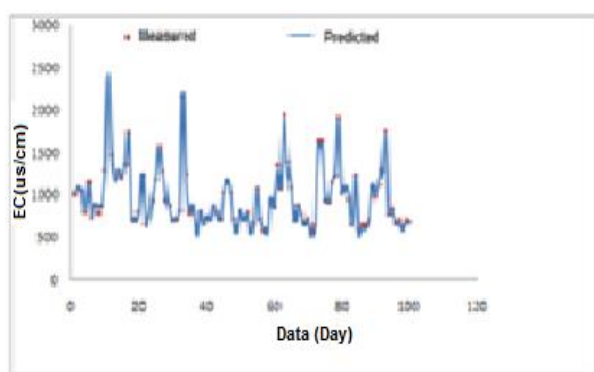


(a) Ahwaz station

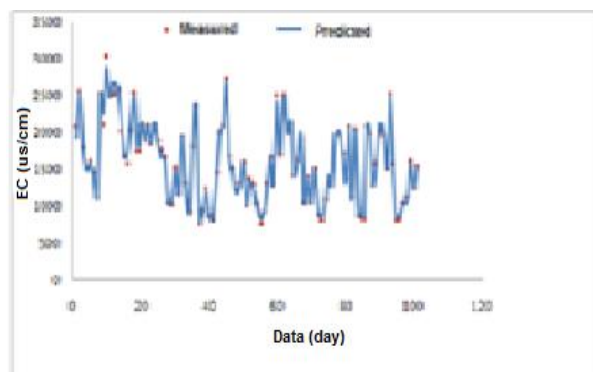


(b) Gotvand station

Figure 4: Comparison of predicted and measured DO values in river water for training and validation sets using ANN model



(a) Ahwaz station



(b) Gotvand station

Figure 5: Comparison of the predicted and measured EC levels in the river water for training and validation sets using ANN model

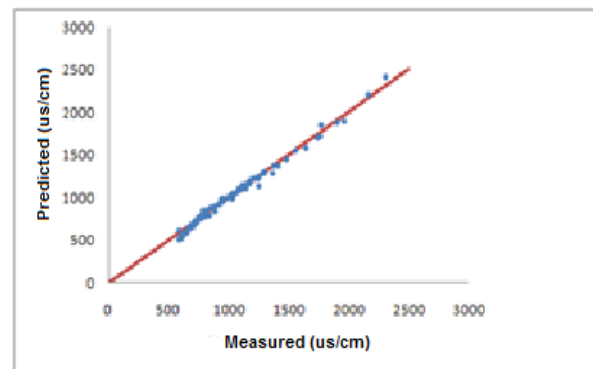
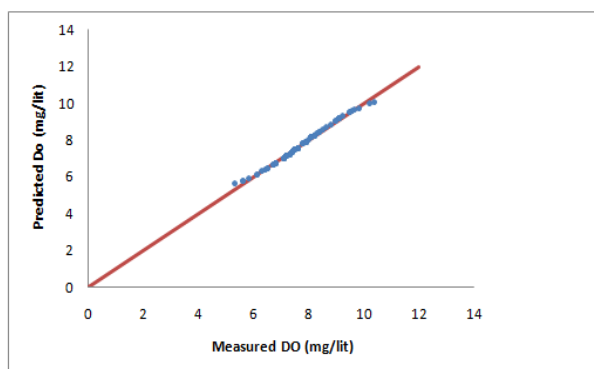


Figure 6: Dispersion diagram of real values versus predicted DO (a) and EC (b) values for test data obtained using ANN model at Ahwaz station

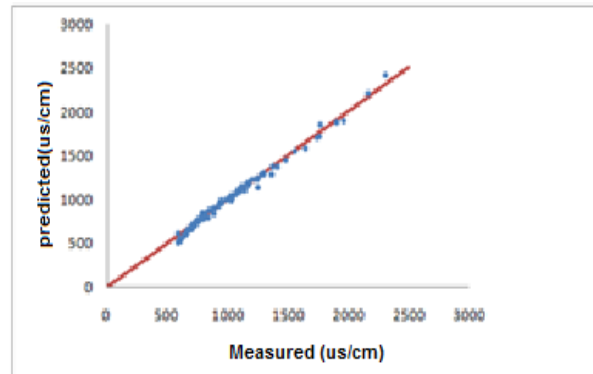
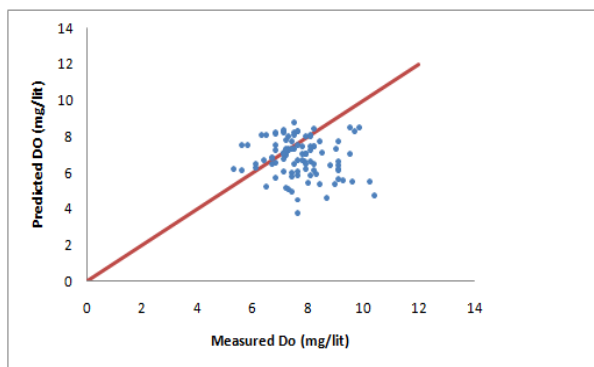


Figure 7: Dispersion diagram of real values versus predicted DO (a) and EC (b) values for test data obtained using ANN model at Gotvand station

The plot between the measured and calculated valences of EC by ANN in training and confirmation sets is indicated in figure 5(a, b). figure 6(a, b) is demonstrating the diffused plots of concrete versus predicted valences of DO and EC which was gained by using ANN models. It is also manifesting the portable achievement of a mediocre plausible agreement between the simulations and observations. Accordingly, the outcomes are showing us that the neural network model has the capability of recognizing the pattern of water quality parameters. Therefore, it can produce a suitable prediction of the monthly change and conversion of water quality data of the Karun River. It can be said that diagram 4 and figure 6 are illustrating the capacity and the capability of the neural network models for predicting the monthly valences of the DO and EC at the Ahwaz and Gatvand stations.

One of the major specifications of a river is water quality even though when it is not used to supply human water. Accordingly, evaluation of the surface water quality is substantial in hydro-environmental management [31]. In modeling and data analysis with ANN plenty of surveys have been done. As an instance: McKnight et al. [32] have represented an ANN model which could approximate the quality of surface water parameters by the usage of some given (available) parameters. The outcomes have shown that the technique of factor analysis was recommended to diagnose water quality parameters. It has been demonstrated that biochemical oxygen demand (BOD), ammonia, nitrogen, Cu, Zn, and Pb have been the most significant parameters for the evaluation of water quality variation in the case of study. The project was well-found on GB3838 "Environmental standards for surface water.

4 Conclusion

There's a one-layer network as a model which is using the Hopfield Neural Network algorithm and also it has been created by MATLAB. Diamantopoulou et al. [43] have shown a model by the use of data from one of Axioms river quality monitoring situations. Above mentioned data has been used as input data for training a feed-forward neural network and it was gathered from 1980 to 1944. Such parameters as temperature, flow, EC, HC0_3 , S0_4 , Na, Cl, Ca, and DO were input data in the reported model and nitrate was the output.

As it is well-known the ANN model can be used in plenty of experimental practical and scientific projects. We have expected this because of the nonlinear character and nature of the transfer function similar to DO, EC, and some other water quality parameters that were among water quality characteristics. In this research, it has been shown that the optimal networks can obtain long-term trends which were apperceived for the tedious water quality variables (DO, EC) in both time and space. In this survey, we have focused on the ANN model and especially the capability of this model to simulate river water quality data. The outcomes have shown us that the usage and demand of this water model are beneficial in any of the following cases: (1) An appropriate gadget for the approximation of the missing data (2) Calibration of evaluation gadgets (3) The susceptibility to predict quality data (4) Adequate for situations with experimental obstacles (5) An accurate embedment for customary equations. These outcomes have shown the neural network's ability to detect the pattern of water quality parameters and provide appropriate forecasts of monthly changes in water quality data (DO and EC) of Karun River. We would suggest neural networks as efficient gadgets for the calculation of river water quality. It also can be used for

a better comprehension tendency in other zones. Hence this model could be considered as a potential predictive alternative to other customary modeling techniques.

Competing interests

The authors declare that no conflict of interest would prejudice the impartiality of this scientific work.

Authors' contribution

All authors of this study have a complete contribution to data collection, data analyses, and manuscript writing.

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