

RESEARCH PAPER

Use of ANFIS/Genetic Algorithm and Neural Network to Predict Inorganic Indicators of Water Quality

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Abstract

The present research used novel hybrid computational intelligence (CI) models to predict inorganic indicators of water quality. Two CI models i.e. artificial neural network (ANN) and a hybrid adaptive neuro-fuzzy inference system (ANFIS) trained by genetic algorithm (GA) were used to predict inorganic indicators of water quality including total dissolved solids (TDS), total hardness (TH), total alkalinity (TAlk), and electrical conductivity (σ). The study was conducted on samples collected from water wells of Kermanshah province through analyzing water parameters including pH, temperature (T), and the sum of mill equivalents of cations (SC) and anions (SA). A multilayer perceptron (MLP) structure was used to forecast inorganic indicators of water quality using the ANN approach. A MATLAB code was used for the proposed ANFIS model to adjust and optimize the ANFIS parameters during the training process using GA. The accuracy of the generated models was described using various evaluation techniques such as mean absolute error (MAE), correlation factor (R), and mean relative error percentage (MRE%). The results showed that both methods were suitable for predicting inorganic indicators of water quality. Moreover, the comparison of the two methods showed that the predicted values obtained from the ANFIS/GA model were better than those obtained from the ANN approach.

Keywords: ANFIS, ANN, Genetic Algorithm, Water Quality

Introduction

To characterize water quality, it is necessary to assess physical, biological, and chemical variables. In general, to investigate the effects of different processes on the quality of water, many plans examine the water quality to provide the required information for the management of water resources [1,2]. Pollution of water resources with chemicals and excessive nutrients results from contamination with wastewater flow containing degradable organics, domestic effluent, agricultural waste, and nutrients [3,4]. Pollution of water resources has become one of the main threats to public and environmental health, thus it is necessary to continuously monitor water resources [5]. The contaminants hurt water quality parameters such as pH, total dissolved solids (TDS), dissolved oxygen (DO) content, conductivity, temperature, transparency, and a viscosity [6–8]. A variety of chemical and biological assessment methods are available but among them, TDS, conductivity, and hardness are the most important parameters for measuring water quality [9–12]. Modeling has widely been used by researchers to predict water quality index (such as pollutant concentrations) based on current water conditions [13,14]. Meanwhile, various water quality models such as traditional mechanistic approaches and artificial neural networks (ANN) have been successfully applied to accomplish the best practices for predicting

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water quality [15–17]. However, these models have some limitations, for instance, they require several input parameters that are not easily accessible; thus, the limitations make the process expensive and time-consuming [18]. Nowadays, ANN and adaptive neuro-fuzzy inference system (ANFIS) are used by many researchers to predict and forecast parameters in various areas like water resources quality assessment [19–21]. These methods are highly accepted because they require less data for forecasting and are more preferred than deterministic models; also, unlike other mathematical models, they do not require a complex and explicit description [22,23].

ANFIS and ANN models were used by Areerachakul [24] to forecast the biochemical oxygen demand (BOD) of the Saen Saep canal in Bangkok. The studied variables which were chosen as inputs included chemical oxygen demand (COD), dissolved oxygen, total coliform bacteria (T-coliform), ammonia nitrogen, and nitrate nitrogen. The experimental results revealed that, as compared with the adaptive ANFIS model, ANN model provided a higher correlation coefficient (R=0.7300 vs. R=0.6768) and a lower mean square error (RMSE%=4.53 vs. RMSE%=4.8182). Yan et al. [25] applied ANFIS model for classifying the water quality status of all major river basins in China in terms of several physical and inorganic chemical indicators including dissolved oxygen, chemical oxygen demand, and ammonia-nitrogen. For training and validating the model, they collected 845 samples from 100 monitoring stations. Moreover, ANN was applied to compare the performance of the models. Recently, Masrur Ahmed and Shah [26] applied ANFIS model to estimate BOD of the Surma River in the northeastern region of Bangladesh. Based on their results, ANFIS model was successfully applied to establish a river water quality prediction model and performed better than other conventional conceptual models. The present study aimed to develop ANN and ANFIS techniques for forecasting inorganic indicators of water quality including hardness, total dissolved solids, conductivity, and alkalinity of water wells of Kermanshah province. The models had four input parameters including pH, temperature, and the sum of mill equivalents of cations and anions. The proposed ANFIS model was trained using the genetic algorithm (GA) to obtain an optimized structure with good accuracy and with the minimum number of membership functions. We combined ANFIS with GA to construct a new model with high levels of accuracy and flexibility and low execution time requirements.

Experimental Method

Kermanshah province is one of the 31 provinces of Iran that is located in the western part of Iran at an approximate latitude of 34.3168 and longitude of 47.0591 with an area of about 24,998 km². Generally, drinking water in rural areas is obtained from water wells, hence, the water quality parameters are monitored using standard methods introduced by the American Public Health Association (APHA). The data set covered 860 observations at different monitoring stations and included four water quality parameters monitored monthly in 2015. The data were obtained from the Rural Water and Sewage Company of Kermanshah province. The measured parameters were pH, temperature, the sum of mill equivalents of cations and anions, alkalinity, hardness, total dissolved solids, and conductivity; the last four parameters were used to construct a water quality model. Fig. 1 shows the data used in this study. The ranges of the selected input/output parameters are presented in Table 1.

Developing the Proposed Models

This study aimed to introduce novel models based on ANN and ANFIS/GA structures to predict the inorganic indicators of water quality. The inputs of CI models included the sum of anions

(SA), the sum of cations (SC), temperature (*T*), and pH. The outputs included electrical conductivity (σ), total dissolved solids (TDS), total hardness (TH), and total alkalinity (TAlk).



Fig. 1. Data used in this study; a) sum of anions, b) sum of cations, c) temperature, d) pH, e) electrical conductivity, f) total dissolved solids, g) total hardness, and h) total alkalinity

Table 1. Input and output variables of the models							
Input/Output	Variable	Variable name	Unit	Range			
	SA	Sum of anions	meq/L	3.20-19.41			
Inputs	SC	Sum of cations	meq/L	3.16-11.32			
	Т	Temperature	°Č	17.70-26.90			
	pН	pH	-	7.3-8			
	σ	Electrical conductivity	μs/cm	321-1849			
Outout	TDS	Total dissolved solid	mg/L	199.02-1146.38			
Output	TH	Total hardness	mg CaCO ₃ /L	186-570			
	Talk	Total alkalinity	mg CaCO ₃ /L	174-332			

Artificial neural network

ANN structure is based on the biological neural network operation [27]. The artificial neuron is the basic processing element of ANN, in which the synapses of biological neurons are modeled as weights. Using the back-propagation algorithm, which is an error-minimization method, the weights can be adjusted. The multi-layer perceptron (MLP) network is one of the widely used ANN structures. As shown in Fig. 2a, MLP has at least three layers; i.e. input layer,

an output layer, and one or more hidden layers [28]. Each layer in MLP structure has several neurons. In Fig. 2a $X_1, X_2, ..., X_n$ are the inputs, $Y_1, Y_2, ..., Y_m$ are the outputs, n is the number of inputs, and m is the number of outputs. In this figure, the output of t^{th} neuron in the hidden layer is given by the following equation:

$$\theta_t = f\left(\sum_{k=1}^n (X_k W_{kt}) + b_t\right) \qquad t = 1, 2, \dots, i$$
(1)

where f is the hidden layer activation function (usually tansig function), b is the bias term, and W is the weighting factor. Also, the output of j^{th} neuron in the output layer is given by the following equation:

$$y_{i} = \sum_{k=1}^{n} (\theta_{k}W_{kj}) + b_{j} \qquad j = 1, 2, ..., m$$

$$(2)$$

$$x_{n} \rightarrow y_{i} \qquad y_{m} \qquad y_{m}$$

Adaptive Neuro-Fuzzy Inference System

ANFIS has the advantages of both the fuzzy system and ANN network. It is a fuzzy inference system (FIS) implemented using ANN [29,30]. Fig. 2b shows the ANFIS structure. Each ANFIS structure has five layers described as follow:

Layer 1: Every node in this layer is an adaptive node with a node function given by:

$$\begin{array}{ll}
O_{1,i} = \mu_{A_i}(x) , & i = 1, 2 \\
O_{1,i} = \mu_{B_{i-2}}(y) , & i = 3, 4
\end{array} \tag{3}$$
(4)

where *i* is the membership grade of a fuzzy set (A_1, A_2, B_1, B_2) , and $O_{1,i}$ is the output of the node *i* in layer 1. Gaussian function is a typical membership function (MF) given by Eq. 5.

$$\mu_A(x) = \exp(-\frac{(x-c)^2}{2\sigma^2})$$
(5)

In Eq. 5 *c* and σ are called nonlinear parameters (premise parameters).

Layer 2: The fixed nodes in this layer multiply all incoming signals and represent the firing strength of a rule. The outputs of the nodes in this layer are given by Eq. 6.

i

$$O_{2,i} = w_i = \mu_{A_i}(x)\mu_{B_i}(y)$$
, $i = 1, 2$ (6)

Layer 3: The fixed nodes in this layer calculate the ratio of the i^{th} rule's firing strength to the sum of all rule's firing strengths given by:

$$O_{3,i} = \overline{w_i} = \frac{w_i}{w_1 + w_2}$$
, $i = 1, 2$ (7)

Layer 4: The outputs of adaptive nodes in this layer is given by:

$$O_{4,i} = \overline{w_i} f_i = \overline{w_i} (p_i x + q_i y + r_i) \quad , \quad i = 1, 2$$

$$\tag{8}$$

Layer 5: The fixed node in this layer has an output function given by:

$$O_{5,i} = \sum_{i} \overline{w_i} f_i = \frac{\sum_{i} w_i f_i}{\sum_{i} w_i} \quad , \quad i = 1, 2$$
⁽⁹⁾

Modeling Approach

In general, several parameters influence the inorganic indicators of water quality (electrical conductivity, total dissolved solids, total hardness, and total alkalinity). The effects of the sum of anions, sum of cations, temperature, and pH on these parameters are investigated. Accordingly, accurate models based on ANN and ANFIS structures were presented to model and predict the effect of input parameters on the inorganic indicators of water quality. In these CI models, the input parameters were defined as the sum of anions, the sum of cations, temperature, and pH. Moreover, electrical conductivity, total dissolved solids, total hardness, and total alkalinity were considered as the output parameters of the models.

The data set required to train and test the proposed CI models were obtained from the water wells of Kermanshah province. The total number of samples used to develop the CI models was 860. 70% and 30% of all the samples were used for training and testing, respectively. MATLAB software was used to develop the proposed models. To obtain the best models, different ANN and ANFIS configurations were trained and tested. To obtain the best ANN structure, many different structures tested one to three hidden layers. Also, the number of neurons in each hidden layer changed from 1 to 9, and for each MLP structure, the number of epochs changed from 100 to 550. To obtain the best ANFIS models, input membership function type (Triangular-shaped, Trapezoidal-shaped, Gaussian, etc.), the number of input membership functions (2 to 12), and the number of training epochs (50 to 500) were changed. Then, the GA parameters such as maximum iterations, population size, crossover probability, mutation probability, mutation rate, etc. were determined. Afterward, the GA fitness function was formulated. The optimization problem has the values of the premise and consequent parameters, and the number of membership functions as the decision variables. Finally, ANN and ANFIS structures were trained and tested through testing and training the data. The specifications of the best proposed ANN and ANFIS/GA models are shown in Tables 2 and 3, respectively.

Table 2. Characteristics of the best proposed MLP model					
No. of hidden layers	2				
No. of neurons in the input layer	4				
No. of neurons in the first hidden layer	5				
No. of neurons in the second hidden layer	8				
No. of neurons in the output layer	4				
Learning rate	0.5				
Number of epochs	200				
Learning function	Trainlm				
Activation function	Tansig				

For the proposed ANFIS models trained by GA, the following parameters were used in GA: crossover percentage=0.7, mutation percentage=0.5, mutation rate=0.1, and selection pressure=8. TrainIm is an ANN training function that updates values of weights and biases based on the Levenberg-Marquardt (LM) algorithm. Also, the learning rate is an important parameter in the process of training MLP networks; it can be changed to confirm that the weights converge fast enough to obtain a response without producing oscillations.

Table 3. Specification of the best ANFIS/GA models						
Specification	Proposed ANFIS models					
Specification	σ	TDS	TH	TAlk		
Туре	Sugeno	Sugeno	Sugeno	Sugeno		
Inputs/outputs	4/1	4/1	4/1	4/1		
No. of MFs for each input	5	3	4	5		
No. of output MFs	5	3	4	5		
Input MF type	Gaussian	Gaussian	Gaussian	Gaussian		
Output MF type	linear	Linear	linear	linear		
No. of fuzzy rules	5	3	4	5		
No. of nonlinear parameters	80	48	64	80		
No. of linear parameters	25	15	20	25		
No. of iterations	1000	650	600	500		
No. of populations	50	80	80	150		

Result and Discussion

The comparison between the proposed ANN and ANFIS/GA models and the experimental data for training and testing are shown in Figs. 3 and 4, respectively. Figs. 3a and 4a show the predicted results of ANN and ANFIS/GA models as compared with the experimental data on electrical conductivity. Moreover, the same plots for total dissolved solids, total hardness, and total alkalinity are shown in Figs. 3b and 4b, Figs. 3c and 4c, and Figs. 3d and 4d, respectively. As shown, ANFIS/GA model was more accurate than the ANN model to follow the outputs in both training and testing data.

To show a better comparison between the proposed ANN and ANFIS/GA models, we used four standard error functions i.e. MRE% (mean relative error percentage), RMSE (root mean square error), CF (correlation factor), and MAE (mean absolute error). The following equations define these standard errors:

MRE % = 100 ×
$$\frac{1}{N} \sum_{i=1}^{N} \left| \frac{x_{i_{exp}} - x_{i_{pred}}}{x_{i_{exp}}} \right|$$
 (10)

$$RMSE = \left[\frac{\sum_{i=1}^{N} \left(x_{i_{exp}} - x_{i_{pred}}\right)^2}{N}\right]^{3/3}$$
(11)

$$CF = 1 - \left[\frac{\sum_{i=1}^{N} \left(x_{i_{exp}} - x_{i_{pred}} \right)^2}{\sum_{i=1}^{N} \left(x_{i_{exp}} \right)^2} \right]$$
(12)

$$MAE = \frac{1}{N} \sum_{i=1}^{N} \left| x_{i_{exp}} - x_{i_{pred}} \right|$$
(13)

where ' $x_{i_{exp}}$ ' and ' $x_{i_{pred}}$ ' are the experimental data and predicted values (ANN or ANFIS), respectively, and N is the number of data. Table 4 shows the overall errors obtained for the proposed models as compared with the experimental data. These errors are obtained for both

training and testing data. As shown in Table 4, the proposed ANFIS/GA models are capable to predict the electrical conductivity, total dissolved solids, total hardness, and total alkalinity, outputs better than the proposed ANN model. Fig. 5 shows a better comparison between the experimental data and the ANFIS/GA models used for training and testing the data. As shown in these figures, it is clear that the obtained results using the ANFIS/GA models are close to the experimental data.



Fig. 3. Comparison of ANN model with the experimental data



Fig. 4. Comparison of ANFIS/GA models with the experimental data



Fig. 5. Results obtained from the ANFIS models a, b, c, and d) training data; e, f, g, and h) testing data

			Error			
Network	Output	Data	MRE%	MAE	RMSE	CF
ANN	_	Training	8.804	44.749	59.043	0.961471
	σ	Testing	9.511	46.592	59.902	0.932712
	TDC	Training	8.806	27.751	36.599	0.961489
	TDS	Testing	9.499	28.852	37.107	0.932849
	TU	Training	5.951	15.143	18.980	0.940413
	TH	Testing	6.601	16.5490	20.321	0.898696
	T A 11-	Training	6.522	15.229	19.308	0.851623
	TAlk	Testing	6.934	15.9651	19.706	0.836748
ANFIS/GA	_	Training	3.375	17.042	22.813	0.994418
	σ	Testing	3.428	17.386	23.158	0.990580
	TDS	Training	3.426	10.754	14.332	0.994300
		Testing	3.528	11.062	14.978	0.989887
	TU	Training	3.233	8.441	11.969	0.976760
	TH	Testing	3.241	8.305	10.998	0.971598
	TAlk	Training	3.985	9.499	12.603	0.939709
		Testing	4.194	9.921	12.878	0.934787

Table 4. Errors of the best proposed ANN and ANFIS/GA

Conclusion

This paper aimed to use an artificial neural network and a novel hybrid computational intelligence model for predicting inorganic indicators of water quality. The proposed ANFIS/GA model combines the genetic algorithm and ANFIS methods. There was a satisfactory level of consistency between the constructed models and the experimental values. The comparison between the results showed that the proposed ANFIS/GA approach was an accurate promising tool with a better result as compared with ANN method. Therefore, ANFIS/GA is a method that can be used to solve more complex scientific and technological problems. Also, the introduced models can provide an insight into some instructions to predict new inorganic indicators of water quality.

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