Adaptive neuro fuzzy inference system for classification of water quality status

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Abstract

An adaptive neuro fuzzy inference system was used for classifying water quality status of river. It applied several physical and inorganic chemical indicators including dissolved oxygen, chemical oxygen demand, and ammonia-nitrogen. A data set (nine weeks, total 845 observations) was collected from 100 monitoring stations in all major river basins in China and used for training and validating the model. Up to 89.59% of the data could be correctly classified using this model. Such performance was more competitive when compared with artificial neural networks. It is applicable in evaluation and classification of water quality status.

Key words: adaptive neuro fuzzy inference system; artificial neural networks; water quality status; classification

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Introduction

Water quality assessment plays an important role in environmental management and decision-making and it provides a scientific basis for rational utilization and protection of water resources. Traditional methods hardly address the non-linearity, subjectivity, and complexity of the cause-effect relationships between water quality variables and water quality status, and there is no a generally accepted method so far. Some methods are usually employed to evaluate the water quality status, including fuzzy synthetic evaluation (Liu et al., 2009; Zou et al., 2006), matter element model (Wang et al., 2004), logistic curve model (Jin et al., 2003), Gray analysis method (Zhang et al., 2004), attribute recognition model (Wang and Zou, 2008) and artificial neural networks (ANN). Among them, the ANN method is regarded as a potentially useful tool for modeling complex non-linear systems and has been widely used for water quality classification and evaluation (Zou and Wang, 2007; Sun et al., 2004; Guo et al., 2000).

New techniques such as fuzzy logic (FL) and adaptive neuro fuzzy inference system (ANFIS) have been recently used as efficient alternative tools for modeling of complex water resources systems and widely used for forecasting. FL is a rule based system consisting of three conceptual components, including (1) a rule-base, containing a selection of fuzzy if-then rules; (2) a data-base, defining the membership functions used in the fuzzy rules; (3) an inference system, performing the inference procedure upon the rules to derive an output (Fig. 1) (Zhang, 2009). FL models focus on the use of heuristics in the system description. The models can be seen as logical models that use if-then rules to establish qualitative and quantitative relationships among variables. Their rule-based nature allows the use of information expressed in the form of natural language statements, making the model transparent for interpretation (Vernieuwe et al., 2005). However, the main problem with FL is that there is no systematic procedure to define the membership function parameters, which must be predetermined by expert knowledge about the modeled system. The construction of the fuzzy rule necessitates the definition of premises and consequences as fuzzy sets. At the same time, ANN has the ability to learn from input and output pairs and adapt to it in an interactive manner. In order to overcome the problems, the ANFIS method, which integrates ANN and FL was proposed by Jang (1993). ANFIS has the potential to capture the benefits of both the methods in a single framework. ANFIS eliminates the basic problem in fuzzy system design (defining the membership function parameters and obtaining a set of fuzzy if-then rules) by effectively using the learning capability of ANN for automatic fuzzy if-then rule generation and parameter optimization (Nayak et al., 2004). Since the concept of ANFIS was first introduced in 1993 (Jang, 1993), it has successfully been proved in many engineering applications such as rainfall-runoff and real-time reservoir operation (Chen et al., 2005; Chang and Chang, 2006; Firat and Gündoğur, 2007).

The purpose of the present study was to develop a model based on ANFIS and evaluate the applicability of the ANFIS approach to assess and classify water quality status, and compare the performance with ANN. This article is organized as follows: Section 1 presents the study area and water quality data, architecture and the hybrid learning algorithm of an ANFIS with a simple illustration. Section
2 presents comparisons of the performance for the different models. The last section contains some concluding remarks.

1 Materials and methods

1.1 Study area and water quality data

The National Environmental Monitoring Center of China (CNEMC) has been monitoring various water quality parameters from 100 automatic water quality monitoring stations, which cover almost all major river basins in China, including Songhua River, Liaohe River, Haihe River, Huaihe River, Yellow River, Yangtze River, Pearl River, Taihu Lake, Chaohu Lake, Dianchi Lake, Qiantang River, and Minjiang River.

In the present study, the data set, covering 845 observations and comprising 3 water quality parameters monitored weekly over nine weeks from 40th to 48th week in 2009, were obtained from CNEMC (http://datacenter.mep.gov.cn/getCountGraph.do?type=runQianWater). The selected water quality parameters, including dissolved oxygen (DO), chemical oxygen demand (COD) and ammonia-nitrogen (NH$_3$-N) were adopted to construct the water quality classification model.

1.2 Methodology of ANFIS

1.2.1 Architecture of ANFIS

ANFIS is a multilayer feed-forward network that uses neural network learning algorithms and fuzzy logic to map an input space to an output space. Five layers are used to construct this inference system. Each layer contains several nodes described by the node function. Adaptive nodes, denoted by squares, represent the parameter sets that are adjustable in these nodes, whereas fixed nodes, denoted by circles, represent the parameter sets that are fixed in the system. The output data from the nodes in the previous layers will be the input in the present layer. There are two types of fuzzy inference system (FIS) described in the literature (Mamdani and Assilian, 1975; Takagi and Sugeno, 1985). The most important difference between the two systems is the definition of the consequence parameter. The consequence parameter in Sugeno FIS is either a linear equation, called “first-order Sugeno FIS”, or constant coefficient, “zero-order Sugeno FIS” (Jang et al., 1997). The Sugeno FIS is used in the present study.

To illustrate the procedures of the ANFIS, for simplicity, it is assumed that the system includes two inputs, DO and COD, and one output, water quality status (WQS). Suppose that the rule base contains two fuzzy if-then rules. For the first-order Sugeno FIS: the two rules can be expressed as:

Rule 1:
If DO is $A_1$ and COD is $B_1$,
then $f_1 = p_1 \times DO + q_1 \times COD + r_1$

Rule 2:
If DO is $A_2$ and COD is $B_2$,
then $f_2 = p_2 \times DO + q_2 \times COD + r_2$

where, $p_i$, $q_i$ and $r_i$ ($i = 1, 2$) are the linear parameters in the consequent part of the Sugeno fuzzy model. The architecture of ANFIS is shown in Fig. 2, and a brief introduction of the model is as follows:

**Layer 1**: input notes. Each node in this layer generates membership grades of the crisp inputs and each node’s output $O_i^1$ is calculated by Eq. (1)

$$O_i^1 = \mu_{A_i}(DO) \quad i = 1, 2; \quad (1)$$

$$O_i^1 = \mu_{B_i}(COD) \quad i = 3, 4 \quad (2)$$

where, DO and COD are the crisp inputs to the node $i$, $A_i$ and $B_i$ are the linguistic labels characterized by appropriate membership functions $\mu_{A_i}$ and $\mu_{B_i}$, respectively. The Guassian membership function is used in this study.

$$\mu_{A_i}(DO) = e^{-\frac{(DO - b_i)^2}{2a_i^2}} \quad (3)$$

$$\mu_{B_i}(COD) = e^{-\frac{(COD - c_i)^2}{2b_i^2}} \quad (4)$$

where, $\{a_i, b_i, c_i\}$ is the parameter set of the membership functions in the premise part of fuzzy if-then rules that

![Diagram of ANFIS](https://example.com/ANFIS_diagram.png)

Fig. 2 Architecture of ANFIS.
change the shapes of the membership functions. Parameters in this layer are referred to as the premise parameters.

Layer 2: rule nodes. The outputs of this layer, called firing strengths \( O_i \), are the products of the corresponding degrees obtained from the layer 1.

\[
O_i = w_i = \mu_A(\text{DO})\mu_B(\text{COD}), \quad i = 1, 2
\]  

(5)

Layer 3: average nodes. The main objective of this part is to calculate the ratio of each \( i \)th rule’s firing strength to the sum of all rules’ firing strength. Consequently, \( \bar{w}_i \) is taken as the normalized firing strength.

\[
\bar{O}_i = \bar{w}_i = \frac{w_i}{\sum_i w_i}, \quad i = 1, 2
\]  

(6)

Layer 4: consequent node. The node function of the fourth layer computes the contribution of each \( i \)th rule’s toward the overall output and the function defined as

\[
O_i = \bar{w}_i f_i = \bar{w}_i (p_i \times \text{DO} + q_i \times \text{COD} + r_i), \quad i = 1, 2
\]  

(7)

where, \( \bar{w}_i \) is the output of layer 3, and \( \{p_i, q_i, r_i\} \) is the parameter set. Parameters in this layer are referred to as consequent parameters.

Layer 5: output node. The single node computes the overall output by summing all the incoming signals. Accordingly, the defuzzification process transforms each rule’s fuzzy results into a crisp output in this layer.

\[
\bar{O}^* = \text{WQS} = \sum_i \bar{w}_i f_i = \frac{\sum_i w_i f_i}{\sum_i w_i} 
\]  

(8)

1.2.2 Estimation of parameters

From the ANFIS architecture presented in Fig. 2, we know that if the premise parameters \( \{a, b\} \) are fixed, the overall output can be expressed as linear combinations of consequent parameters \( \{p, q, r\} \). More precisely, the output can be rewritten as,

\[
\text{WQS} = \sum_i \bar{w}_i f_i = \bar{w}_1 f_1 + \bar{w}_2 f_2 = (\bar{w}_1 \text{DO})p_1 + (\bar{w}_1 \text{COD})q_1 + \bar{w}_1 r_1 + (\bar{w}_2 \text{DO})p_2 + (\bar{w}_2 \text{COD})q_2 + \bar{w}_2 r_2
\]  

(9)

Suppose that the given training data set has entries. Let matrices

\[
B = \begin{bmatrix}
\text{WQS}_1 \\
\text{WQS}_2 \\
\vdots \\
\text{WQS}_m
\end{bmatrix}, \quad X = \begin{bmatrix}
p_1 \\
q_1 \\
r_1 \\
p_2 \\
q_2 \\
r_2
\end{bmatrix}
\]  

(10)

and

\[
A = \begin{bmatrix}
\bar{w}_1 \text{DO} & \bar{w}_1 \text{COD} & \bar{w}_1 \\
\bar{w}_2 \text{DO} & \bar{w}_2 \text{COD} & \bar{w}_2 \\
\vdots & \vdots & \vdots \\
\bar{w}_m \text{DO} & \bar{w}_m \text{COD} & \bar{w}_m
\end{bmatrix}
\]

Then, based on \( m \) entries of training data \( \{\text{DO}_i, \text{COD}_i, \text{WQS}_i\} \), given the values of the premise parameters \( \{a, b\} \), Eq. (8) can be expressed in matrix form as:

\[
AX = B
\]  

(11)

where, \( X \) is an unknown matrix, whose elements come from the consequent parameters set. This is a standard linear least squares problem, thereby the least squares estimator (LSE) \( X^* \) is given by Eq. (10)

\[
X^* = (A^T A)^{-1} A^T B
\]  

(12)

where, \( A^T \) is the transpose of \( A \), and \( A^{-1} \) is the inverse of \( A \).

ANFIS applies the hybrid learning algorithm, which consists of the combination of “gradient descent” and “least-squares” methods to update the model parameters. Each epoch of this hybrid learning procedure is composed of a forward pass and a backward pass. In the forward pass of the hybrid learning procedure, the node output goes forward until layer 4 and the consequent parameters are identified by the least squares method. In the backward pass, the error signal propagates backwards and the premise parameters are updated by gradient descent. A detailed description of this algorithm were introduced by Jang and Sun (1995).

The computation of the data for ANFIS was conducted using the software Matlab. The ANFIS training algorithms, including the gradient method and the least squares method, were embedded in the software of Matlab’s fuzzy inference toolbox. We can use the ANFIS training function in the toolbox for the training with the input data. After training, an ANFIS model with forecasting function will be obtained for output forecasting.

1.2.3 Model development

There are no fixed rules for developing an ANFIS model, even though a general framework can be followed based on previous successful applications in engineering. The goal of ANFIS is to generalize the relationship of the form:

\[
Y = f(X_1, X_2, \ldots, X_n)
\]  

(13)

where, \( X_1, X_2, \ldots, X_n \) are input variables; \( Y \) is the output variable.

In current study, the water quality status (WQS) can be characterized as a function of DO, COD and \( \text{NH}_3\text{-N} \). The relationship between water quality status and input variables can be expressed by

\[
\text{WQS} = f(\text{DO, COD, NH}_3\text{-N})
\]  

(14)

The data in ANFIS are usually divided into three sets: training set, checking set, and testing set. The training data are used for the training of ANFIS, while the checking data are used for verifying the identified ANFIS which prevents over-fitting networks. The testing data are used to evaluate the model performance. In this study, the water quality data (9 weeks, total of 845 observations) were divided into three data sets. The first data set containing 80% of the records was used as the training data; the second data set containing 10% of the records was used as the checking data; while the remaining 10% data were applied as the testing data.
1.2.4 Model verification

The performance of ANFIS models were evaluated according to statistical criteria such as correlation coefficient (CORR), Nash-Sutcliffe coefficient of efficiency (NSCE) (Nash and Sutcliffe, 1970; Benyahya et al., 2007), and root mean square error (RMSE).

\[
\text{CORR} = \frac{\sum_{i=1}^{N} (\text{WQS}_O - \text{WQS}_O)(\text{WQS}_P - \text{WQS}_P)}{\sqrt{\sum_{i=1}^{N} (\text{WQS}_O - \text{WQS}_O)^2(\text{WQS}_P - \text{WQS}_P)^2}}
\]

(15)

\[
\text{NSCE} = 1 - \frac{\sum_{i=1}^{N} (\text{WQS}_O - \text{WQS}_P)^2}{\sum_{i=1}^{N} (\text{WQS}_O - \text{WQS}_O)^2}
\]

(16)

\[
\text{RMSE} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (\text{WQS}_O - \text{WQS}_P)^2}
\]

(17)

where, \(\text{WQS}_P\) is the estimated value, \(\text{WQS}_O\) is the observed value; \(\bar{\text{WQS}}_P\) is the average of estimated values, \(\bar{\text{WQS}}_O\) is the average of observed values. The correlation coefficient is a commonly used statistic and provides information on the strength of linear relationship between the observed and the estimated values. The NSCE is a statistic employed to evaluate model performance. Values of CORR and NSCE close to 1.0 indicate good model performance. The RMSE statistic indicates a model’s ability to predict a value away from the mean.

2 Results and discussion

According to the Environmental Quality Standards for surface water (GB3838-2002), the water quality of rivers was classified into six classes: Class I, II, III, IV, V and under Class V. In this study, 1, 2, 3, 4, 5 and 6 were assigned to the 6 classes as the theoretical output values, respectively. Thus, according to the principle of membership, the range of the model output values corresponding to Class I–V and under Class V should be (0, 1.50), (1.50, 2.50), (2.50, 3.50), (3.50, 4.50), (4.50, 5.50) and > 5.50, respectively. Hence, the output value 1.8 corresponds to Class II, 3.2 to Class III, and 7.4 to the under Class V accordingly.

The ANFIS (Fig. 3) used in this study contained eight rules, with two membership functions being assigned to each input variable. Different membership function types including generalized bell, Gaussian, trapezoidal, triangular, sigmoidal and Pi were tested. The number of linear and non-linear parameters to be optimized is displayed in Table 1. Optimum parameters were found once checking data error reached the minimum. The performance of ANFIS models with different membership functions are also given in Table 1.

As seen in Table 1, for the entire data set, CORR, NSCE and RMSE with ANFIS models were in the ranges from 0.3435 to 0.9665, –2.8031 to 0.9430 and 0.3338 to 2.5564, respectively. For the testing data set, the same indices were in the ranges from 0.2974 to 0.9689, –1.9550 to 0.9316 and 0.3704 to 2.4341, respectively. Obviously, the performance of model 2 is better than those of other models. The CORR and NSCE values of model 2 are higher than those of other models and RMSE value of model 2 is smaller than those of other models either for entire data set or testing data set. In addition, the correctly classified points of model 2

---

**Table 1** Performance of ANFIS models with different membership functions

<table>
<thead>
<tr>
<th>Model</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Membership function</td>
<td>Generalized bell</td>
<td>Gaussian</td>
<td>Two Gaussian</td>
<td>Trapezoidal</td>
<td>Triangular</td>
<td>psigmf**</td>
<td>dsigmf**</td>
<td>pimf**</td>
</tr>
<tr>
<td>Parameters</td>
<td>Linear</td>
<td>32</td>
<td>32</td>
<td>32</td>
<td>32</td>
<td>32</td>
<td>32</td>
<td>32</td>
</tr>
<tr>
<td></td>
<td>Non-linear</td>
<td>18</td>
<td>12</td>
<td>12</td>
<td>24</td>
<td>18</td>
<td>24</td>
<td>24</td>
</tr>
<tr>
<td>CORR</td>
<td>0.9611</td>
<td>0.9665</td>
<td>0.9492</td>
<td>0.9474</td>
<td>0.9499</td>
<td>0.3435</td>
<td>0.3471</td>
<td>0.9505</td>
</tr>
<tr>
<td>NSCE</td>
<td>0.9225</td>
<td>0.9340</td>
<td>0.8963</td>
<td>0.8972</td>
<td>0.9021</td>
<td>–2.8730</td>
<td>–2.8031</td>
<td>0.9016</td>
</tr>
<tr>
<td>RMSE</td>
<td>0.3616</td>
<td>0.3338</td>
<td>0.4184</td>
<td>0.4165</td>
<td>0.4065</td>
<td>2.5564</td>
<td>2.5333</td>
<td>0.4075</td>
</tr>
<tr>
<td>Correctly classified points</td>
<td>757</td>
<td>757</td>
<td>748</td>
<td>678</td>
<td>679</td>
<td>686</td>
<td>686</td>
<td>692</td>
</tr>
</tbody>
</table>

* DEV-1*, predicted water quality status has resulted one level lesser than real; *DEV+1*, predicted water quality status has resulted one grade higher than real; total points, 845.
** psigmf: product of two sigmoid membership functions; dsigmf: membership function composed of the difference between two sigmoidal; pimf: Pi-shaped curve membership function.
is 757 which is the largest in all models. As a result, the best fitting model was obtained with the FIS composed by Gaussian membership function. Figure 4 shows the rules for the ANFIS model, respectively.

Figure 5 compares the results of the best model and observation data. The verifications results indicate that the model estimated results reasonably match the observed water quality status. CORR, NSCE and RMSE for entire data set and testing data set are 0.9665 and 0.9689, 0.9340 and 0.9316, 0.3338 and 0.3704, respectively, which are satisfactory in common model applications.

In order to assess the ability of the ANFIS model relative to that of a neural network model, an ANN model was constructed using the same input parameters to the ANFIS model. A standard back propagation algorithm was employed for training, and the hidden neurons were optimized by trial and error. The final ANN architecture consists of seven hidden neurons. The ANN model was trained using the same training data set as used for the ANFIS. The performances of ANN and ANFIS in terms of the performance indices are presented in Table 2.

As shown Table 2, although the performance of both the ANFIS and the ANN models are similar either for entire data set or testing data set in terms of CORR, NSCE, RMSE, the ANFIS shows a slight improvement over the ANN in terms of correctly classified points and percentage of correctly classified points. The weak point of ANN occurred during the testing stage. When ANN was asked for predicting the water quality status for the testing data set composed by 85 samples, only 78.82% were correctly classified. However, the ANFIS correctly classified the 91.76% of the testing points, demonstrating the higher generalization skills of the ANFIS model.

The proposed method in this study was applied only physical and inorganic chemical parameters. The method decreased the three quality values to one synthetic value as an index in continuous form, which enables river water quality assessment more comprehensible. For instance, although the index values of 1.8 and 2.2 both represent the Class II, we can easily conclude that the former water quality status is better than the latter. This method can also be used for the other parameters like organic parameters, inorganic pollution parameters and bacteriologic parameters.

3 Conclusions

Applicability of ANFIS approach for water quality status assessment and classification was investigated. Eight
models with different membership functions were constructed and trained by ANFIS methods. Comparing the performance of models, the ANFIS model with Gaussian membership function had the best performance and was selected as the best fitting model. The highest value of CORR and NCSE and the lowest value of RMSE were obtained from the ANFIS model. The model was verified with 845 sample points of various rivers. As a result, the model can correctly predict 89.59% of the river quality status, which demonstrated satisfactory results of this new approach. This model performed better than ANN model and can generate output value in continuous form which makes water quality assessment more comprehensible.

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