Shallow groundwater quality assessment: use of the improved Nemerow pollution index, wavelet transform and neural networks

Q. Yang, J. Zhang, Z. Hou, X. Lei, W. Tai, W. Chen and T. Chen

ABSTRACT

Shallow groundwater is generally of great interest to the community due to its easy availability. However, it is very sensitive to external stimulus. In this paper, shallow groundwater quality is assessed and classified with improved Nemerow pollution index, multi-layer perceptron artificial neural network (MLP-ANN) optimized with a back-propagation algorithm and wavelet neural network (WNN) methods in a coastal aquifer, Fujian Province, South China. The data used in three models were collected during the pre-monsoon over the period 2004–2011. The eight parameters, total dissolved solids, total hardness, chemical oxygen demand, chloride, sulphate, nitrate, nitrite and fluorides, were selected to characterize groundwater quality classification based on the National Quality Standard for Groundwater (GB/T 14848-93). The results of MLP-ANN and WNN are interpreted by mean absolute error, root mean square error and R^2 (determination coefficient) criteria. The results obtained from three methods demonstrate that WNN has a higher accuracy compared with the other two methods. The study reveals that these methods are efficient tools for assessing groundwater quality.

Key words | groundwater quality assessment, Nemerow pollution index, neural network, wavelet transform

Q. Yang (corresponding author)
J. Zhang
Z. Hou
W. Tai
W. Chen
Key Laboratory of Groundwater Resources and
   Environment Ministry of Education,
Jilin University,
Changchun 130021,
China
E-mail: qyang@jlu.edu.cn

X. Lei
China Institute of Water Resources and
   Hydropower Research,
Beijing 010000,
China

T. Chen
Electric Power Research Institute, Jilin Electric
   Power Co., Ltd of State Grid,
Changchun 130021,
China

INTRODUCTION

Water quality assessment is a complex problem due to multiple factors involved, and difficulties of accurate identification of the pollution components which are affected by many factors and processes. The groundwater quality depends not only on natural factors such as the lithology of the aquifer, the quality of recharge water and the type of interaction between water and aquifer, but also on human activities, which can alter these groundwater systems either by polluting them or by changing the hydrological cycle (Helena *et al.* 2000). Pollutant issues in water sources because of human activity have been of great concern in recent years (Nash & McCall 1995; UNEP 'the United Nations Environment Programme' 1999; Milovanovic 2007; Mohapatra *et al.* 2011; Ogunkunle & Fatoba 2013). Various methods in groundwater quality assessment have been explored. Types of water quality indices were applied in

environmental assessment (Wayne 1978; Li *et al.* 2007; Lermontova *et al.* 2009; Ni *et al.* 2010; Liang *et al.* 2011; Tang *et al.* 2011; Sarala & Sabitha 2012; Ma *et al.* 2013). Many traditional approaches and techniques have been applied to water quality assessment including multivariate statistical methods such as cluster analysis, factor analysis, principal component analysis and discriminant analysis, which generally were used to identify the major factors affecting groundwater. The use of graphical methods such as the Stiff diagram (Stiff 1951) to interpret the hydrochemistry is limited to two dimensions (Hem 1970). However, due to the complex nonlinear relationships and uncertainties between the parameters on groundwater quality, artificial neural networks (ANNs) have become a popular method in environmental simulation and prediction because they can overcome some of the difficulties associated with traditional

statistical approaches (Wu *et al.* 2009; Chen *et al.* 2015; Gholami *et al.* 2015; Taormina & Chau 2015; Wang *et al.* 2015).

According to a review paper of ANN applications to water resource variables that had been published until the end of 1998 (Maier & Dandy 2000), the authors reviewed 43 papers and reported that in these papers surface water flow and quality was the topic in 28 and rainfall forecasting in 13 (Yang *et al.* 2015). The application of ANNs in assessing groundwater quality in recent years has been reported in several studies (Aris *et al.* 2012; Khashei-Siuki & Sarbazi 2013; Nadiri *et al.* 2013; Pedro *et al.* 2013). One of the most important features of ANN models is their ability to adapt to recurrent changes and detect patterns in a complex natural system (Cannas *et al.* 2006; Adamowski 2007; Partal 2009; Tiwari & Chatterjee 2010; Adamowski & Chan 2011). Application of ANN in hydrological forecasting and prediction can be traced back to the 1990s, ANN models are called 'black box' models due to their ability to model dynamic nonlinear systems by detecting patterns in a complex system, without the need to understand the physical mechanism taking place in the system. ANNs are proven to be effective in modeling virtually any nonlinear function to a desired degree of accuracy. The advantages of ANN models over conventional simulation methods have been discussed in detail by French *et al.* (1992). The most popular type of ANN is the multi-layer perceptron (MLP) model optimized with a backpropagation (BP) algorithm. However, a problem solved with ANNs and other non-linear methods is that they have some limitations with non-stationary data if pre-processing of the input data is not conducted. In the last decade, wavelet analysis has been applied in water resources engineering and hydrology, and it has been found to be very effective for handling non-stationary data. Wavelet transforms can decompose the original time series, and the wavelet-transformed data improve the ability of a forecasting model by capturing useful information on various resolution levels (Adamowski & Sun 2010).

The main advantages of ANN can be summarized as follows: (1) high efficiency of computation in dealing with large quantities of data and nonlinear relationship between parameters (especially for water quality) and data transfer during the calculation process, which enable its accuracy in water quality assessment or simulation; (2) memory ability of large capacity can store large volumes of water quality data and the corresponding relationship between inputs and outputs, combination of high speed of computation will inevitably enhance intelligence level of water quality assessment and simulation; (3) learning ability avoids some processes such as mechanism analysis, boundary and initial hypothesis, parameter estimation and calibration in establishing groundwater quality simulation, only model training is necessary to determine the input–output relationship, which greatly simplifies the model setup procedure.

The main purpose of this paper is to construct the improved Nemerow pollution index (INPI) method, MLP-ANN and wavelet neural network (WNN) methods and demonstrate their applicability to assess and classify the shallow groundwater quality. Comparison among these three methods can provide useful insights for identifying the effectiveness of each method.

DATA AND METHODOLOGY

Groundwater quality dataset

The groundwater quality data of five boreholes were obtained by monitoring the ion concentrations at Dongshan hydrological station, including total dissolved solids (TDS), the total hardness (TH), permanganate, chloride, fluoride, nitrate, nitrite, sulfate. The monitoring period continued from 2004 to 2011, with a total of 320 samples data. Dongshan town is a coastal island located at the most southerly point of 'golden delta' of Fujian Province, lying between $117°17'E–117°35'$ E longitude, $23°33'$ N–$23°47'$ N latitude, consisting of Dongshan island and 44 small islands, and covers an area of about 248.34 km^2 (Figure 1). The total length of coastline is around 200 km. The study area is influenced by the subtropical marine monsoon climate. The annual average temperature is about 20.9°C and varies between 13.1°C in January and 27.3 °C in July. Annual average rainfall is about 1,224.9 mm, most of which occurs during May and September. A typical feature in the study area is frequent typhoons during July and September. Rural population accounts for approximately 80% of the total population. Due to the topography, the
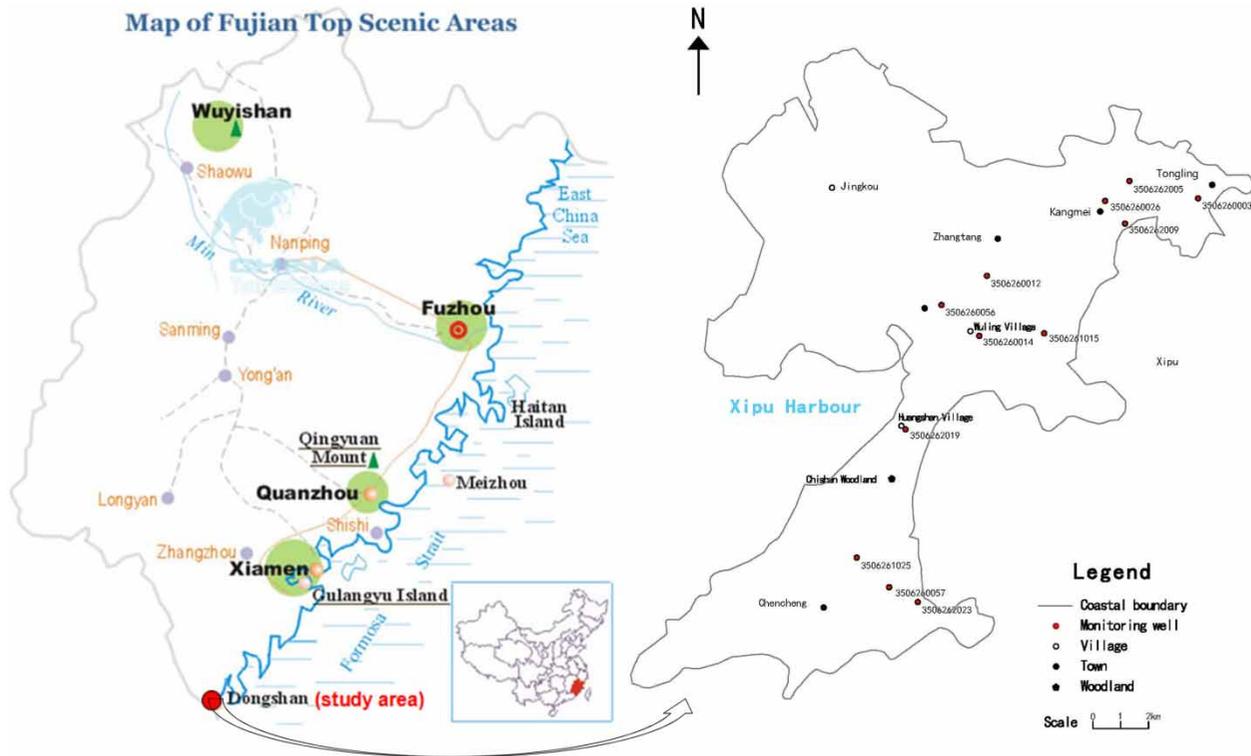
Figure 1 │ Outlined location map of the study area and well locations.

water body is not well developed within Dongshan town, surface water is scarce, and groundwater has become a dependent source of water supply and servers in many aspects. The selected groundwater quality data of five boreholes were obtained by sampling the water and monitoring the ion concentrations with ion chromatograph in summer and post-monsoon seasons (two times, once a year) according to the standard methods for examination of ground water and wastewater at Dongshan hydrological station, which covers pH, TH, TDS, Ca^{2+}, Mg^{2+}, Na^+, Cl^-, SO_4^{2-}, HCO_3^-, NO_3^-, Mn. In this study, the data monitored in summer were used.

The study area can be considered as an independent hydro-geological unit due to the sea surrounding all the four sides. Water yield property differs greatly because of lithology and thickness of the aquifer. Groundwater type is coarse porous water, recharged predominantly by rainfall infiltration.

The INPI method

In scientific stream pollution analysis (Nemerow 1974), the Nemerow pollution index was defined based on the ratio

of the maximum concentrations of pollutant in water to environmental standards and the measured mean value (Chen *et al.* 2012). The index is defined as:

$$P_j = \sqrt{\frac{F_{max}^2 + \bar{F}^2}{2}} \tag{1}$$

where P_j stands for the Nemerow index; $F_{max} = \max \{c_i/s_{ij}\}$, $i = 1, 2, \ldots, n$, $j = 1, 2, \ldots, m$. $\bar{F} = \sum_{i=1}^{n} c_i/s_{ij}/n$, s_{ij} is the standard ion concentration, c_i is the measured ion concentration of water sample. When $c_i/s_{ij} > 1$, $c_i/s_{ij} = 1 + p'\lg(c_i/s_{ij})$ and $p' = 5$. Otherwise, c_i/s_{ij} equals the actual value. The parameters such as the TH, TDS, chemical oxygen demand (COD), Cl^-, SO_4^{2-}, NO_3^-, NO_2^-, F^- are included in the calculation. The water is distributed into three classes according to the method used: the direct use, the indirect use and the none-contact use. The total Nemerow pollution index 'P' ($P = W_1P_1 + W_2P_2 + W_3P_3$) is obtained as a weighted average by statistical analysis.

The assessment of groundwater quality was conducted using multivariate indexes, which gives priority to the

extreme values and weights, as well as the usage purposes of water. The weights are determined according to various uses for the same water. Three essential factors, the water quality indexes, the assessment method and the extreme values and weights, have to be considered in the water quality assessment in the Nemerow pollution index method.

The INPI ranks the groundwater quality classes in accordance with the amount of pollution factors and the standard limits of each quality grade. The improved approach not only considers the effects of pollutants with the maximum pollution degree, but also takes into account the influence of the most dangerous pollution factor in water during the assessment. In other words, the impact of the maximum weights, the second-maximum of weights and the second-maximum of the ratio is of great importance in the evaluation. The improved method calculates the maximum of the ratio and weight via:

$$P_j = \sqrt{\frac{F'^2_{\max} + \bar{F}^2}{2}} \tag{2}$$

where F'_{max} is computed as $F'_{max} = (F_{max} + F_w)/2$, P_j represents the INPI, F_w (considered as the ratio of the maximum of weight) indicates the hazard caused by the most dangerous pollution factor for water quality.

The improved formula considers the second-maximum weight and the second-maximum ratio with:

$$P''_j = \sqrt{\frac{F''^2_{max} + \bar{F}^2}{2}} \tag{3}$$

$$P'''_j = \sqrt{\frac{F'''^2_{max} + \bar{F}^2}{2}} \tag{4}$$

where $F''_{max} = (F_{max} + F_{w1} + F_{w2})/3$, $F'''_{max} = (F_{max1} + F_{max2} + F_{w1} + F_{w2})/4$. The improved method applies statistical analysis with different weights for both the measured values and the standard values in water. P''_j is the INPI after adding the second-maximum of weights. P'''_j is the INPI after adding the second-maximum ratios. F_{w1} and F_{w2} are computed as c_i/s_{ij} of the maximum and second-maximum of weights, respectively. F_{max1} and F_{max2} are computed as c_i/s_{ij} of the maximum and second-maximum of ratios, respectively.

The determination of weights follows the principle of the larger risk and the greater weight. According to the standard for pollutant discharge, the following subsequence is given: S_1, S_2, ..., S_i, ..., S_n. k_i is provided as the correlation of the ratio, where $k_i = S_{max}/S_i$. The weight w_i is calculated as:

$$w_i = \frac{k_i}{\sum_{i=1}^n k_i} \left(\sum_{i=1}^n w_i = 1 \right) \tag{5}$$

In this paper, a computation between the measured concentrations of water samples and standard values prescribed in groundwater quality standards (GB/T14848-93) was firstly carried out, and then the INPI of each grade was obtained. Lastly, the grades of water quality on the basis of the pollution index values were evaluated.

WNN method

WNN, a newly rising mathematical analysis model which combines the wavelet transform with the ANN, has been applied widely in water quality assessment (Dogan *et al.* 2009; Singh *et al.* 2009; Moustris *et al.* 2010; Chu *et al.* 2013). Wavelets are mathematical functions that give a time-scale representation of the time series and their relationships to analyze time series that contain non-stationarities. Wavelet analysis allows the use of long time intervals for low frequency information and shorter intervals for high frequency information and is capable of revealing aspects of data like trends, breakdown points, and discontinuities that other signal analysis techniques might miss. Another advantage of wavelet analysis is the flexible choice of the mother wavelet according to the characteristics of the investigated time series (Adamowski & Sun 2010).

A typical structure of BP neural network topology is shown in Figure 2. It can be seen in Figure 3 that $X_1, X_2, ..., X_k$ are the input parameters, $Y_1, Y_2, ..., Y_m$ are the predicted outputs and ω_{ij} and ω_{jk} are the weights of the WNN. When the input signal sequence is $x_i(i = 1, 2, ..., k)$, the formula of the output in hidden layer is:

$$h(j) = h_j\left(\frac{\sum_{i=1}^k \omega_{ij}x_i - b_j}{a_j}\right) j = 1, 2, \cdots, l \tag{6}$$
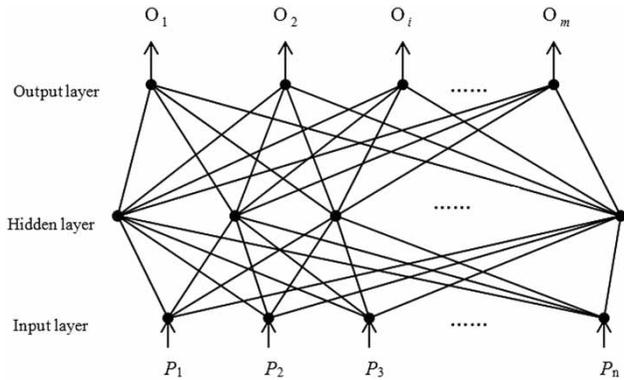
Figure 2 | Configuration of the BP neural network topology.

where $h(j)$ is the output of jth node in the hidden layer; ω_{ij} is the connection weight of the input and hidden layers; b_j is the displacement factor of h_j; a_j is the stretch factor of h_j; and h_j is the wavelet basis function.

When the Morlet wavelet is adapted as the mother wavelet, the mathematical equation is written as:

$$y = \cos(1.75x)e^{-x^2/2}.$$

and the output function of WNN is computed as:

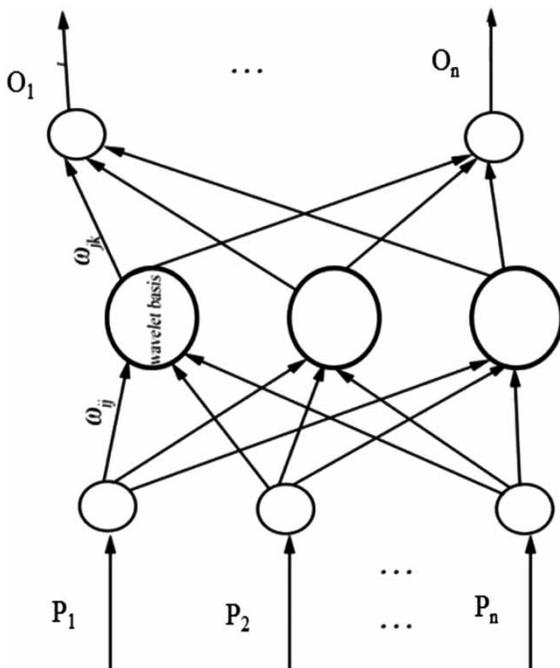$$y(k) = \sum_{i=1}^{l} \omega_{ij} h(i) k = 1, 2, \cdots, m \qquad (7)$$

Figure 3 | WNN architecture.

ω_{ij} is the weight from hidden layer to output layer; $h(i)$ is the output of the ith node in the hidden layer; l is the nodes number in the hidden layer; and m is the nodes number in the output layer.

The weights correction method of WNN is similar to the BP neural network. By adjusting the weights and factors of the wavelet basis in the gradient modification, the output of WNN will approximate to the predicted output. The modification procedure of the WNN process is summarized as follows.

(1) Calculate the predictive error:

$$e = \sum_{k=1}^{m} yn(k) - y(k) \qquad (8)$$

$yn(k)$ is the predictive output; $y(k)$ is the output of WNN.

(2) Adjust weights and factors of wavelet basis according to the predictive error:

$$\omega_{n,k}^{(i+1)} = \omega_{n,k}^{i} + \Delta\omega_{n,k}^{(i+1)}$$

$$a_k^{(i+1)} = a_k^i + \Delta a_k^{(i+1)}$$

$$b_k^{(i+1)} = b_k^i + \Delta b_k^{(i+1)}$$

$\Delta\omega_{n,k}^{(i=1)}$, $\Delta a_k^{(i=1)}$ and $\Delta b_k^{(i=1)}$ are calculated according to the predictive error:

$$\Delta\omega_{n,k}^{(i+1)} = -\eta \frac{\partial e}{\partial \omega_{n,k}^i}$$

$$\Delta a_k^{(i+1)} = -\eta \frac{\partial e}{\partial a_k^i}$$

$$\Delta b_k^{(i+1)} = -\eta \frac{\partial e}{\partial b_k^i}$$

η is the learning rate.

A series of steps are involved in the WNN training:

1. The initialization of networks which contains the parameters such as the weights, the factors of wavelet basis and learning rate.
2. The classification of samples. The samples are grouped into two parts: the training and the testing samples. The training samples are used to train the network and the testing samples are used to test the precision.
3. The prediction of WNN model. Input the trained data, then calculate the predictive output and error.

4. The adjustment of the weights and factors of wavelet basis according to the error.
5. The judgment on whether the algorithm ends. Otherwise, return to step 3.

Model performance indices

Three standard statistical indices, root mean square error (RMSE), determination coefficient (R^2) and mean absolute error (MAE) are employed to evaluate the performances of the WNN model. RMSE evaluates the residual between the observed and forecasting value. MAE measures the MAE between the observed and predicted values. The closer the R^2 value is to 1, the more accurate the model is. The nearer the RMSE and MAE values are to 0, the more accurate the model is. The best fit between observed and calculated values will be obtained with R^2 as 1 and RMSE as 0:

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N}(y_o - y_f)^2}{N}} \tag{9}$$

$$R^2 = \left| \frac{\sum_{i=1}^{N}(y_o - \bar{y}_o)(y_f - \bar{y}_f)}{\sqrt{\sum_{i=1}^{N}(y_o - \bar{y}_o)^2 \sum_{i=1}^{N}(y_f - \bar{y}_f)^2}} \right|^2 \tag{10}$$

$$MAE = \frac{\sum_{i=1}^{N}|y_o - y_f|}{N} \tag{11}$$

where N is the total number of value, y_o is the observed value, y_f is the predicted value, $\bar{y}_o$ is the average of observed values and $\bar{y}_f$ is the average of the predicted value.

RESULTS AND DISCUSSION

Groundwater quality assessment in INPI

In this study, the Grade III standard in the National Quality Standard for Groundwater (GB/T 14848-93) is taken as the assessment criterion. Equation (5) is applied to compute the weights of each selected pollution parameter and the result is summarized in Table 1.

Table 1 | Statistics summary of values of the weights of eight groundwater parameters

Groundwater parameters	Grade III	Weights (W_i)
TH (mg/L)	≤450	4.32×10^{-5}
COD (mg/L)	≤3.0	6.49×10^{-3}
TDS (mg/L)	≤1,000	1.95×10^{-5}
Cl^- (mg/L)	≤250	7.78×10^{-5}
SO_4^{2-} (mg/L)	≤250	7.78×10^{-5}
NO_3^- (mg/L)	≤20	9.73×10^{-4}
NO_2^- (mg/L)	≤0.02	0.973
F^- (mg/L)	≤1.0	0.0195

TH, Total hardness; COD, Chemical oxygen demand; TDS, Total dissolved solids.

Table 2 shows the conversion of the groundwater quality standard from the concentration to the special weights. It can be seen from Table 2 that a water sample with P_j''' less than 0.47643 will be classed into Grade I, which is considered as clean and excellent for drinking. If the concentrations of very few parameters exceed the limits, those water samples are classified as Grade II. Likewise, water samples classified as Grade III mean they are slightly polluted with a few values exceeding the standards. Similarly, water samples in Grade IV mean moderately contaminated with at least two parameters exceeding the criteria. Grade V means the water is seriously polluted as almost all the parameters are far beyond the standard values.

Table 2 | Statistics summary of the improved Nemerow pollution indices in GB/T 14848-93

Groundwater parameters	Grade I	Grade II	Grade III	Grade IV	Grade V
TH (mg/L)	≤150	≤300	≤450	≤550	>550
COD (mg/L)	≤1.0	≤2.0	≤3.0	≤10	>10
TDS (mg/L)	≤300	≤500	≤1,000	≤2,000	>2,000
Cl^- (mg/L)	≤50	≤150	≤250	≤350	>350
SO_4^{2-} (mg/L)	≤50	≤150	≤250	≤350	>350
NO_3^- (mg/L)	≤2.0	≤5.0	≤20	≤30	>30
NO_2^- (mg/L)	≤0.001	≤0.01	≤0.02	≤0.1	>0.1
F^- (mg/L)	≤1.0	≤1.0	≤1.0	≤2.0	>2.0
P_j'''	≤0.476	≤0.702	≤1	≤3.198	>3.198
Water class	Excellent	Good	Fair	Poor	Very poor

TH, Total hardness; COD, Chemical oxygen demand; TDS, Total dissolved solids; P_j''', Improved Nemerow pollution index.

**Table 3** │ Statistics summary of P_j''' of five wells from 2004 to 2011

	P_j'''							
Well no.	2004	2005	2006	2007	2008	2009	2010	2011
#1	1.019	1.625	1.184	1.611	1.184	1.046	1.04812	2.338
#2	0.425	0.467	0.173	0.125	0.302	0.118	0.33455	0.383
#3	1.682	1.834	1.557	1.593	1.770	2.404	1.53089	1.581
#4	6.107	0.722	1.631	0.958	2.577	2.881	0.68956	0.559
#5	0.734	0.096	0.105	0.176	0.567	0.236	0.59233	1.333

The calculations of P_j''' are summarized in Table 3 for the samples over 8 years. By comparing these calculations with the standard values of P_j''', Figure 4 demonstrates the results of water quality assessment in the INPI method. By using this method, the water quality evaluation of five wells in the study area 8 years in succession also analyzes the temporal variation of water quality. It is shown that Wells 1–3 remain at the same water quality grade respectively over 8 years. Well 4 has a slight change of water quality showing a better tendency year by year. Meanwhile, Well 5 has a sharp fluctuation due to uncertain causes, such as climate, the location of wells, human activities. Also, sampling methods could have some impact on the evaluation which should be taken into consideration. These factors interact in a complex way and result in spatial and temporal variation in groundwater quality parameters. Determination of

processes affecting groundwater quality in a coastal aquifer is very complicated.

Groundwater quality assessment in MLP neural network

The groundwater quality data from 2004 to 2009 are used for training/calibration sets and those from 2010 to 2011 are applied as the testing set. After trials, the goal of error learning is set as 1e-5 (Maier & Dandy 2000). The maximum iteration time is set as 5,000. The step size and the learning rate are set as 50 and 0.01. Figure 5 shows the variation of the error in training process. After the 4998th iteration is finished and the error reaches 0.027, the training process of the BP neural network stopped.
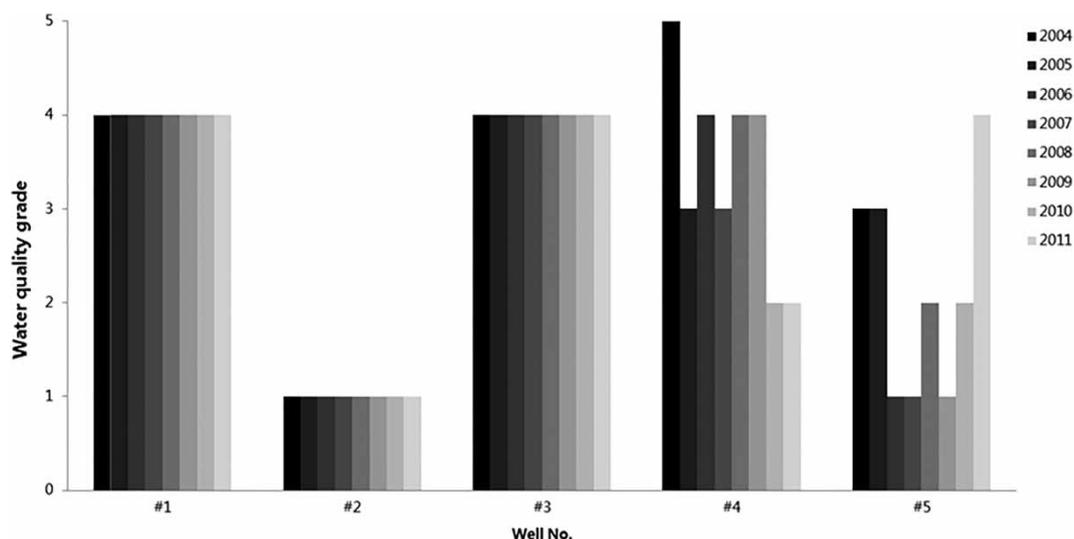
Figure 4 │ Result of groundwater quality assessment in the INPI method.

The eight indicators, TH, COD, TDS, Cl^-, SO_4^{2-}, NO_3^-, NO_2^-, F^-, are selected as eight input vectors. The evaluation grade is treated as the output vector. The structure of the BP neural network is 8-30-1. There are 30 nodes in the hidden layer. By using the neural network function provided by Matlab, a three-layer BP network model is established. Figure 6 shows the comparison of the evaluated and the actual water quality grade in the testing process. The result of the testing process indicates that the model had a good fit.

Groundwater quality assessment in WNN

Data processing

WNN model needs to be trained before it is used to conduct groundwater quality assessment. The selection of the trained samples is of great concern since it is significantly related to the establishment of the WNN model. In this work, the training sample is extracted from the standard data in groundwater environmental quality standards (GB/T14848-93). While all eight indicators are within Grade I, it is identified as Grade I, Grade II is decided while eight indicators are within the Grade II range, and so on. In this study, Latin hypercube sampling (LHS) method was applied for the data sampling. The concept of the Latin-Hypercube simulation is based on Monte Carlo simulation but uses a stratified sampling approach that allows efficient estimation of the output statistics. It subdivides the distribution of each
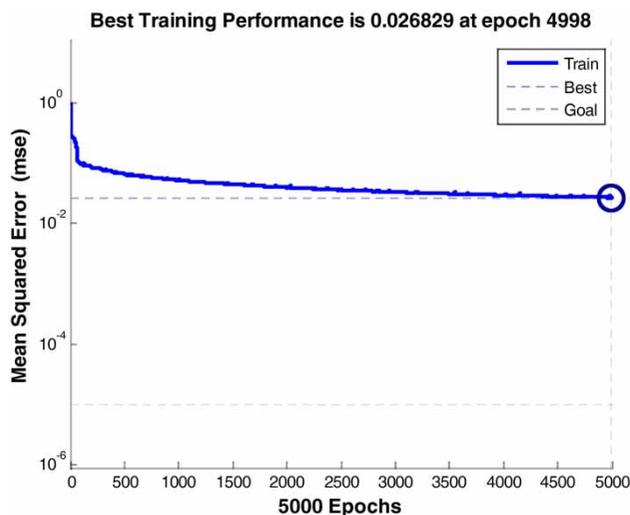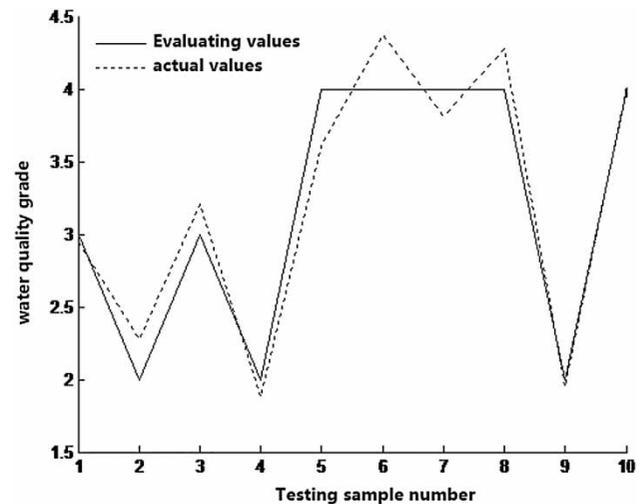

Figure 6 │ Comparison of evaluated and actual water quality grade in BP-ANN.

parameter into N strata with a probability of occurrence equal to 1/N. For uniform distributions, the parameter range is subdivided into N equal intervals. Random values of the parameters are generated such that for each of the P parameters, each interval is sampled only once. This approach results in N non-overlapping realizations and the model is run N times. LHS is commonly applied in water quality modelling due to its efficiency and robustness.

The detailed procedure is summarized as follows: 80 samples are extracted from each grade of water samples, thus a total of 400 samples are applied to train the dataset, and a total of 50 samples are applied to validate the dataset. As eight indicators and one corresponding water quality grade are involved, the sample is a nine-dimensional vector. In this process, Grade I is encoded in the dataset as real number 1; Grade II is encoded as to 2, and so on.

Training and testing

In the training process, eight indicators are set as inputs and the water quality grade is set as the output. Since sometimes the output of WNN is not an integer, it means the output of the WNN model cannot be used for the assessment grade directly. We define water quality grade based on the following rule: when the predicted value is less than 1.5, the sample is identified as Grade I. When the predicted value is greater than 1.5 and less than 2.5, the sample is

Figure 5 │ Error variation in training process within 5,000 epochs.

Table 4 │ WNN model output and its corresponding water quality grade

Output of WNN	y < 1.5	$1.5 \leq y < 2.5$	$2.5 \leq y < 3.5$	$3.5 \leq y < 4.5$	$4.5 \leq y$
Assignment of grade	I	II	III	IV	V

identified as Grade II, and the rest is done in the same manner. Table 4 summarizes these results. Based on the convergence of training error and the matching degree of testing results, the nodes in the hidden layer is determined as 23. After the 2000th iteration, the target error reaches 0.056, and the WNN training process is finished. Figure 7 illustrates the comparison between the evaluated and the actual water quality grade. Obviously the trained WNN model has a higher accuracy by comparing the estimated results with the actual water quality grade. So it is feasible to apply the WNN model for assessing water quality.

Comparative analysis of groundwater quality assessment

To facilitate the comparative water quality assessment results, Table 5 summarizes the assessment results for three methods. The calculated MAE, RMSE and R^2 are 0.292, 0.371, 0.989 for BP-ANN model, and those of WNN are 0.073, 0.091 and 0.996, indicating that WNN model has a higher accuracy. Although the BP model has a good stability shown above, the evaluating result has a relatively large difference. According to the comparison of two neural network methods, the WNN method has a higher accuracy than the BP-ANN method. The BP method requires more iteration with no guarantee of accuracy of the results for the same task. It reveals that the WNN and NMR methods are both effective for water quality assessment because the result is consistent with the actual water quality status.

CONCLUSIONS

In order to assess the groundwater quality in the coastal aquifer, water samples collected during the summer season were investigated in the INPI method, multiple layer perception neural network optimized with back propagation algorithm and wavelet transform neural network. The
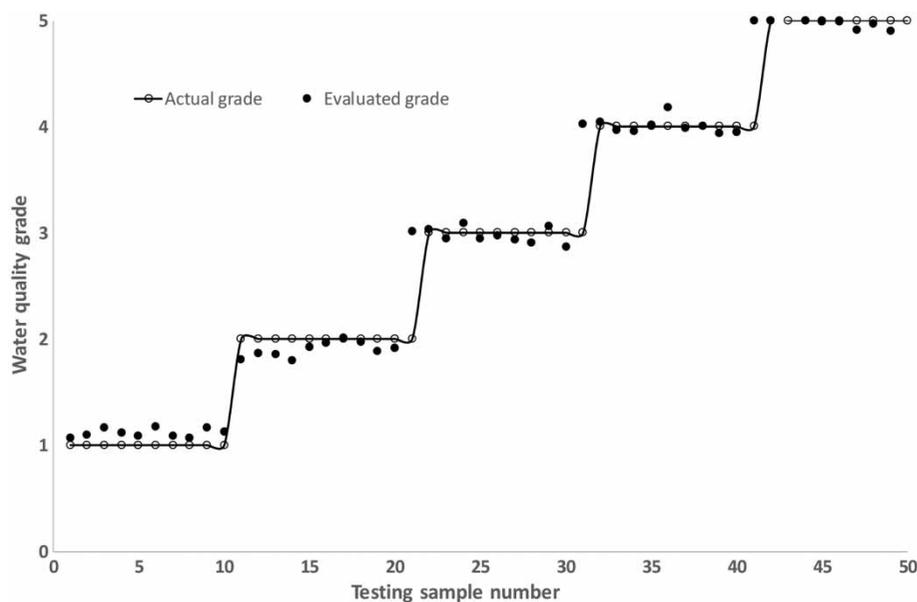

Figure 7 │ Comparison of evaluated and actual water quality grade with WNN.

Table 5 │ Water quality evaluation in the WNN, NMR and BP methods

| | Water quality grade | | | | | | | | | | | | | | |
| | #1 | | | #2 | | | #3 | | | #4 | | | #5 | | |
Year	WNN	NMR	BP	WNN	NMR	BP	WNN	NMR	BP	WNN	NMR	BP	WNN	NMR	BP
2004	IV	IV	III	II	I	III	V	IV	III	I	V	V	II	III	III
2005	IV	IV	IV	II	I	II	IV	IV	III	II	III	IV	I	III	II
2006	IV	IV	V	I	I	IV	V	IV	V	III	IV	IV	I	I	II
2007	IV	IV	III	I	I	II	V	IV	IV	II	III	III	I	I	II
2008	IV	IV	III	I	I	III	V	IV	IV	IV	IV	V	I	II	IV
2009	IV	IV	III	I	I	II	V	IV	IV	IV	IV	V	I	I	III
2010	IV	IV	III	I	I	II	V	IV	III	II	II	II	II	II	IV
2011	IV	IV	V	II	I	III	V	IV	IV	II	II	II	III	IV	IV

NMR, The INPI method.

INPI approach not only considers the effects of pollutants with the maximum pollution degree, but also takes into account the influence of the most dangerous pollution factor including the impact of the maximum weights, the second-maximum of weights and the second-maximum of the ratio, which is of great importance in the evaluation. BP-ANN and WNN both demonstrate good performance in assessing groundwater quality, however, WNN has higher accuracy. To protect shallow water sources from contamination, further study will focus on the exploration about what kinds of pollutants dominantly control the groundwater quality.

Some limitations of the present methods used in this study have to be addressed. The INPI method overestimates the maximum pollution factors. The BP-ANN method, the initial weight and learning rate of hidden layer were artificially determined with experience, therefore the learning process may fall into the local minimum in some cases. Keeping in view the seasonal changes of groundwater chemistry, it is suggested that more water sample data in different seasons and their repeat analysis are required in future work.

ACKNOWLEDGEMENTS

REFERENCES

Adamowski, J. 2007 Development of a short-term river flood forecasting method based on wavelet analysis. *J. Hydrol.* **353** (3–4), 247–266.

Adamowski, J. & Chan, H. F. 2011 A wavelet neural network conjunction model for groundwater level forecasting. *J. Hydrol.* **407**, 28–40.

Adamowski, J. & Sun, K. 2010 Development of a coupled wavelet transform and neural network method for flow forecasting of non-perennial rivers in semi-arid watersheds. *J. Hydrol.* **390**, 85–91.

Aris, Z. S., Praveena, M., Abdullah, H. & Radojevic, M. 2012 Statistical approaches and hydrochemical modelling of groundwater system in a small tropical island. *J. Hydroinform.* **14** (1), 206–220.

Cannas, B., Fanni, A., See, L. & Sias, G. 2006 Data preprocessing for river flow forecasting using neural networks: wavelet transforms and data partitioning. *Phys. Chem. Earth* **31** (18), 1164–1171.

Chen, J., Liu, Q. & Qian, H. 2012 Application of improved Nemerow index method based on entropy weight for groundwater quality evaluation. *Int. J. Environ. Sci.* **2** (3), 1284–1290.

Chen, X. Y., Chau, K. W. & Busari, A. O. 2015 A comparative study of population-based optimization algorithms for downstream river flow forecasting by a hybrid neural network model. *Eng. Appl. Artif. Intell.* **46** (A), 258–268.

Chu, H. B., Lu, W. X. & Zhang, L. 2013 Application of artificial neural network in environmental water quality assessment. *J. Agr. Sci. Tech.* **15**, 343–356.

Dogan, E., Sengorur, B. & Koklu, R. 2009 Modeling biochemical oxygen demand of the Melen River in Turkey using an artificial neural network technique. *J. Environ. Manag.* **90**, 1229–1235.

French, M. N., Krajewski, W. F. & Cuykendall, R. R. 1992 Rainfall forecasting in space and time using a neural network. *J. Hydrol.* **137**, 1–31.

Gholami, V., Chau, K. W., Fadaee, F., Torkaman, F. & Ghaffari, A. 2015 Modeling of groundwater level fluctuations using dendrochronology in alluvial aquifers. *J. Hydrol.* **529** (3), 1060–1069.

Helena, B., Pardo, R. & Vega, M. 2000 Temporal evolution of groundwater composition in an alluvial aquifer (Pisuerga River, Spain) by principal component analysis. *Water Res.* **34** (3), 807–816.

Hem, J. D. 1970 Study and interpretation of the chemical characteristics of natural water. *U.S. Geology Survey Water-Supply Paper*, 3rd edn. United States Government Printing Office, Alexandria, pp. 263.

Khashei-Siuki, A. & Sarbazi, M. 2013 Evaluation of ANFIS, ANN, and geostatistical models to spatial distribution of groundwater quality (case study: Mashhad plain in Iran). *Arab. J. Geosci.* **7** (10), 4175–4190.

Kia, M. B., Pirasteh, S., Pradhan, B., Mahmud, A. M., Sulaiman, W. N. A. & Moraddi, A. 2012 An artificial neural network model for flood simulation using GIS: Johor river basin, Malaysia. *Environ. Earth Sci.* **67** (1), 251–264.

Lermontova, A., Yokoyamab, L. & Lermontov, M. 2009 River quality analysis using fuzzy water quality index: Ribeira do Iguape river watershed, Brazil. *Ecol. Indic.* **9** (6), 1188–1197.

Li, Z., He, Y. J. & Zhu, Z. D. 2007 Application of entropy and weigh method for water quality evaluation in rural area. *Yellow River* **29** (5), 35–37.

Liang, J., Chen, C., Song, X., Hang, Y. & Liang, Z. 2011 Assessment of heavy metal pollution in soil and plant from Dunhua sewage irrigation area. *Int. J. Electrochem. Sci.* **6**, 5314–5324.

Ma, Z., Song, X. F., Wan, R. & Gao, L. 2013 A modified water quality index for intensive shrimp ponds of litopenaeus vannamei. *Ecol. Indic.* **24**, 287–293.

Maier, H. R. & Dandy, G. C. 2000 Neural networks for the prediction and forecasting of water resources variables: a review of modeling issues and applications. *Environ. Modell. Softw.* **15**, 101–124.

Milovanovic, M. 2007 Water quality assessment and determination of pollution sources along the Axios/Vardar River, Southeastern Europe. *Desalination* **213**, 159–173.

Mohapatra, P. K., Vijay, R., Pujari, P. R., Sundaray, S. K. & Mohanty, B. P. 2011 Determination of processes affecting groundwater quality in the coastal aquifer beneath Puri city, India: a multivariate statistical approach. *Water Sci. Technol.* **64** (4), 809–817.

Moustris, K. P., Ziomas, I. C. & Paliatsos, A. G. 2010 3-day-ahead forecasting of regional pollution index for the pollutants NO_2, CO, SO_2, and O_3 using artificial neural networks in Athens, Greece. *Water Air Soil Pollut.* **209**, 29–43.

Nadiri, A. A., Fijani, E., Tsai, F. T.-C. & Asghari Moghaddam, A. A. 2013 Supervised committee machine with artificial intelligence for prediction of fluoride concentration. *J. Hydroinform.* **15** (4), 1474–1490.

Nash, H. & McCall, G. J. H. 1995 *Groundwater Quality: 17th Special Report*. Chapman and Hall, London.

Nemerow, N. L. 1974 *Scientific Stream Pollution Analysis*. McGraw-Hill, New York.

Ni, X., Lu, J., Lan, L., Gao, F. Q. & Pan, C. L. 2010 Interactions between environmental quality and economic development in Shanghai, China. *Int. J. Eng. Sci. Technol.* **2** (7), 56–64.

Ogunkunle, C. O. & Fatoba, P. O. 2013 Pollution loads and the ecological risk assessment of soil heavy metals around a mega cement factory in southwest Nigeria. *Pol. J. Environ. Stud.* **22** (3), 487–493.

Partal, T. 2009 Modelling evapotranspiration using discrete wavelet transform and neural networks. *Hydrol. Process.* **23** (25), 3545–3555.

Pedro, A. A., Antonio, F., Rosa, F. R. & Molina, L. 2013 Groundwater quality assessment using data clustering based on hybrid Bayesian networks. *Stoch. Environ. Res. Risk Assess.* **27**, 435–447.

Sarala, T. D. & Sabitha, M. A. 2012 Calculating integrated pollution indices for heavy metals in ecological geochemistry assessment near Sugar Mill. *J. Res. Biol.* **12** (5), 489–498.

Singh, K. P., Basant, A., Malik, A. & Jain, G. 2009 Artificial neural network modeling of the river water quality: a case study. *Ecol. Modell.* **220**, 888–895.

Stiff, H. A. 1951 The interpretation of chemical analysis by means of patterns. *J. Petrol Technol.* **3**, 15–17.

Tang, T., Zhai, Y. J. & Huang, K. 2011 Water quality analysis and recommendations through comprehensive pollution index method: take Qilu Lake as an example. *Manage. Sci. Eng.* **5** (2), 95–100.

Taormina, R. & Chau, K. W. 2015 Data-driven input variable selection for rainfall-runoff modeling using binary-coded particle swarm optimization and extreme learning machines. *J. Hydrol.* **529** (3), 1617–1632.

Tiwari, M. K. & Chatterjee, C. 2010 Development of an accurate and reliable hourly flood forecasting model using wavelet–bootstrap–ANN (WBANN) hybrid approach. *J. Hydrol.* **1** (394), 458–470.

UNEP 1999 *Global Environment Outlook 2000*. Earthscan Publications, London.

Wang, W. C., Chau, K. W., Xu, D. M. & Chen, X. Y. 2015 Improving forecasting accuracy of annual runoff time series using ARIMA based on EEMD decomposition. *Water Resour. Manage.* **29** (8), 2655–2675.

Wayne, R. O. 1978 *Water Quality Indices: A Survey of Indices Used in the United States*. US Environmental Protection Agency, Washington, DC.

Wu, C. L., Chau, K. W. & Li, Y. S. 2009 Methods to improve neural network performance in daily flows prediction. *J. Hydrol.* **372** (1–4), 80–93.

Yang, Q., Hou, Z., Wang, Y., Zhao, Y. & Martin, J. D. 2015 A comparative study of shallow groundwater level simulation with WA–ANN and ITS model in a coastal island of south China. *Arab. J. Geosci.* **8**, 6583–6593.