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ORIGINAL ARTICLE

Simulation of nitrate contamination in groundwater using artificial neural networks

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Abstract In this study, performance of two artificial networks was evaluated to determine which one would have more efficiency in predicting nitrate contamination of groundwater. The case study was in Babol which is recognized as one of the most fertile regions in Iran. Relevant factors including hydrogeology, soil nitrogen content, soil organic matter and soil carbon content were measured in situ as input data to predict nitrate in groundwater, then correlated by using the Pearson formula. Next, back-propagation and radial basis function neural networks were applied one-by-one. The best structure for back-propagation model was found to be 4-5-1 and Radial basis function with a spread parameter equal to 0.5 and the mean square error (MSE) of 0.50 mg/l. Results showed no significant difference between the proposed models. Both ANN models can reliably predict nitrate contamination in groundwater with acceptable accuracy. However, the radial basis model showed marginally better performance compared to back-propagation by 30 %.

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Introduction

In recent years, groundwater as one of the main sources of drinking water is being exposed to an increasingly serious pollution. Several studies have demonstrated that nitrate nitrogen (NO_3-N) is the most common groundwater pollutant (Ehteshami and Biglarijoo 2014; Rivett et al. 2008). Nitrate in drinking water can cause various types of cancer (Unesian 1990). Therefore, the maximum permissible concentration for drinking water was determined below 10 ppm of NO_3-N in USA, or 45 ppm according to the recommendation of the World Health Organization (Ehteshami et al. 2013).

Being endowed with rich water resources, fertile soil and temperate climate, agriculture is highly developed in northern part of Iran. Consequently, nitrogen fertilizers are used in large amounts and high rates. Several previous researches have studied nitrate pollution in groundwater as well as nitrate concentration of groundwater in local areas, however, with the main focus on general statistic (Alabdula'aly 1997; Bruggeman et al. 1995). Agriculture is one of the human activities that have a large 'ecological footprint', including a significant influence on nitrate contamination of groundwater (Carey and Lloyd 1985; Williams et al. 2014; MacQuarrie et al. 2001). Application of nitrogen fertilizers and nitrate leakage from livestock are two main factors responsible for groundwater quality degradation (Sweeten et al. 1995). Based upon previous studies, there is a direct relation between nitrate contamination in groundwater and agricultural management practices (Follett et al. 1991; Lee et al. 1992; Hinkle and Tesoriero 2014).

In order to study the nitrate concentration in groundwater of Gilan and Mazandaran rice fields, samples of surface and groundwater including water in rice fields, rivers, drains, domestic wells and semi deep wells were analyzed in 1995. Results showed that the most nitrate concentration differences are related to domestic wells and during spring season and almost 3 % of wells contained nitrate contamination, which exceeds the standard level (Malakuti 2000). Unesian (1990) reported to determine nitrate concentration in groundwater in Sari County, 32 samples were collected and analyzed by an ultra violet spectrophotometer and showed the nitrate concentration in 4 % of region wells was more than permissible nitrate level. Most of the studies have used statistical methods such as spatial interpolation.

Since 1990s, artificial neural network (ANN) algorithms has been developed rapidly, and widely used to derive predictive results in hydrologic analysis, water resources and management of agricultural non-point source pollution. Application of artificial neural networks is becoming common to solve various types of engineering prediction and optimization problems (Salami and Ehteshami 2015, 2016). Although some previous studies focused on estimating NO_3 pollution in groundwater, selection of input, type of network and case properties made considerable differences between investigators. The distribution of groundwater NO_3-N pollution is also simulated using neural networks, however, in these studies, the selection of input layers relied on subjective judgments rather than concrete numerical analysis (Strebel et al. 1989; Maithani 2009). The high concentration of NO_3-N in groundwater is ascribed to a multi-factorial dynamic interaction process in intensive farming (Maithani 2009). Strebel et al. (1989) indicated that NO_3-N usually overloads into groundwater as a result of excessive use of nitrogen fertilizers in intensive farming and cropping systems with low N-use efficiency. Therefore, a reliable model should be able to analyze and simulate each influential factor, either natural or anthropological, to accurately determine its contribution in increasing the NO_3-N concentration in groundwater.

Suen and Eheart (2003) collated the effectiveness of Back-propagation neural networks (BPNNs) and radial basis function neural networks (RBFNNs). These two models were also compared with conventional water quality modeling methods such as regression and mechanistic. Concerning overall precision RBFNN outperfomed others.

Sharma et al. (2003) simulated the subsurface drain outflow and nitrate–nitrogen concentration in tile effluent adopting a trainable fast back-propagation (FBP) network and a self-organizing radial basis function (RBF) network. Data were gathered in the period of 40 month and employed to train the models. Supreme performance of the RBF neural network in predicting the concentration of nitrate-nitrogen was confirmed. Moasheri et al. (2013) strived for a more accurate and reliable understanding of spatial distribution of sodium, calcium and magnesium in Kashan aquifer by merging statistical methods and artificial neural networks. Results suggested high precision of the method.

In this study, the Back-Propagation Neural Network (BPNN) and Radial basis (fewer neurons), two popular artificial neural networks is applied to simulate the groundwater nitrate concentration in Babol. The main objective of the study is to investigate the complex non-linear relationship between multi-factorial behaviors of nitrate groundwater contamination.

Materials and methods

Study area

Babol is situated in Mazandaran province. This area encompasses 14,301 km^2 which is about 5.94 % of the Mazandaran province, located between 36°05′ and 36°35′ latitude, and 52°30′ and 52°45′ longitude. A total of 80,900 Ha is under cultivation of rice, fruits, vegetables, grain and other products as it is shown in Table 1. At the same time, the health of groundwater is particularly important, not only because its potable use by the majority of local people but also for its possible interaction with other open water bodies at lower elevations. City of Babol is situated 210 km northeast of Tehran and it is surrounded by Babolsar at north, Alborz Mountains at south, Amol city at west and Ghaemshahr and Savadkooh at east. In this area, shallow wells are the main source of drinking water supply The average water table depth is about 2.5 m with the minimum at the ground surface level while a maximum depth of 5.5 m was observed at the southern part of plain (Badei 1998).

Urea is the most common fertilizer used in the area. Its water solubility and its leaching potential are high enough to contaminate groundwater. High concentrations of nitrate in drinking water can cause drastic diseases such as Methemoglobinemia in infants and stomach cancer in adults (Lee et al. 1992; Wolfe and Patz 2002). A concentration of 10 mg/l is a generally accepted limit for safe drinking water (USEPA 2012). WHO guideline for drinking water proposed the standard level of 50 mg NO_3/l for nitrate concentration in drinking water. USEPA (2012) maximum allowable contaminant levels in drinking water for nitrate and nitrite concentration are 10 mg N/l (=45 mg NO_3/l) and 1 mg N/l, respectively. The rate of fertilizer application in Babol County including urea and phosphates are 13,000 and 4000 tons annually respectively. Therefore, possible consequences of its high usage necessitated us to conduct this study with the objective of accurately

Table 1 Annual usage of urea and phosphate fertilizers in Babol County

Cultivation	Rice	Fruits	Vegetables	Grains	Other products
In acre	50,000	11,000	6500	400	13,000
Urea fertilizer (kg/acre)	200	100	150	150	100
Phosphate (kg/acre)	50	50	–	50	50

assessing its seepage rate and occurrence in local groundwater.

Water sampling

The sampling was performed in fifty randomly selected wells as shown in Fig. 1. The sampling and the associated analyses was conducted in autumn season. The average concentration of nitrate was 20.88 mg/l while the maximum value in rice farm region was 45.5 mg/l, which is less than WHO standard but it is according to USEPA standard out of the acceptable range. The minimum nitrate rate was 4.3 mg/l which was measured in fruit gardens. The water testing was performed using DR2000 Spectrophotometer (by: HACH, USA) at Babol university health service laboratory. The samples transferred to the laboratory in the shortest possible period of time, and analyses were conducted readily. Furthermore, 10 cc of sulfuric acid was added to each sample to preserve its quality.

Soil and water laboratory analyses

From a list of 145 wells in the study area 50 wells were selected randomly, so a uniform grid at the scale of

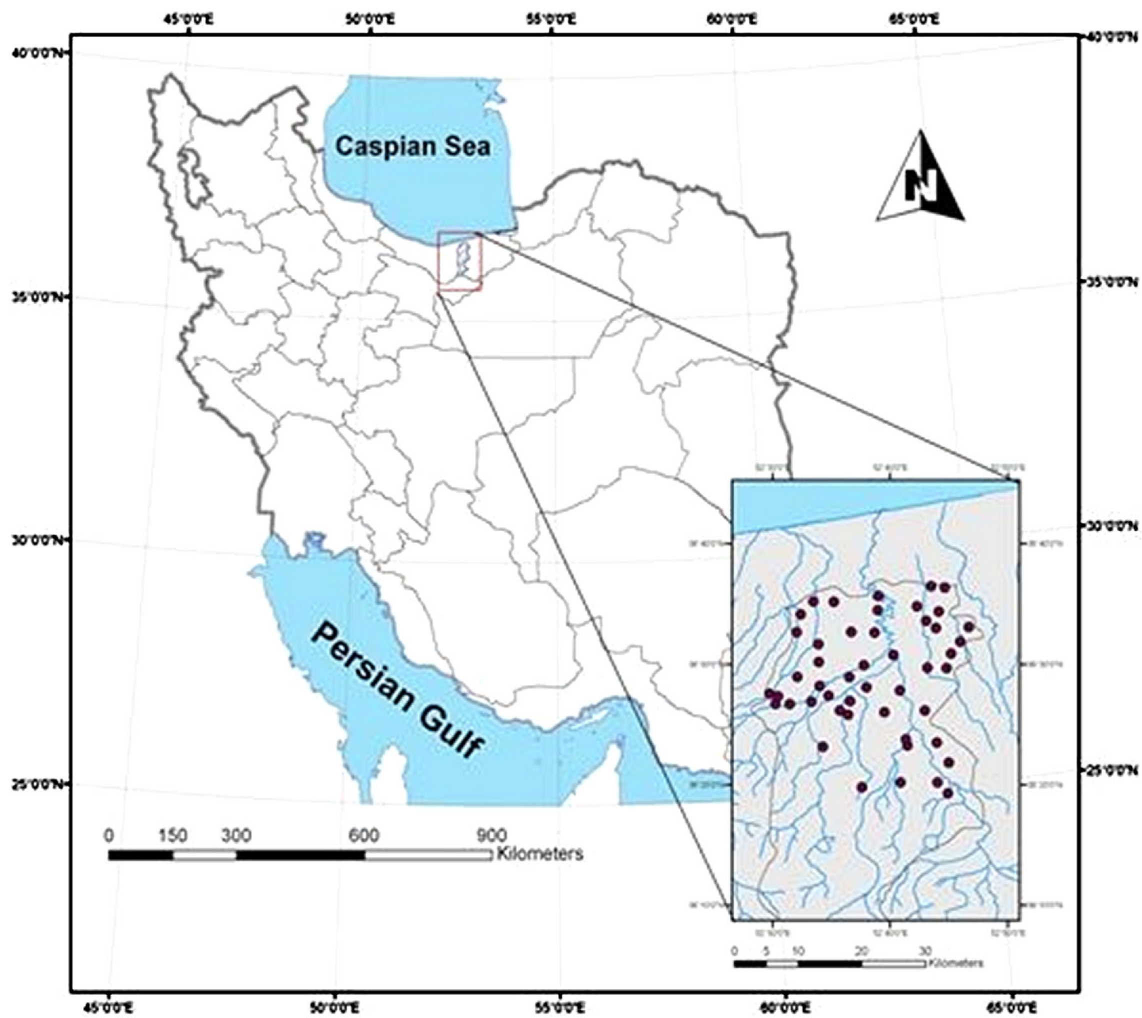

Fig. 1 Study area and sampling distribution in Babol

1 × 1 km were made and adapted to the wells map. The selected wells were within the residential area and mostly in agricultural zones. Autumn was the season to start the sampling for three continuous years. Extended studies indicate that autumn is the best season for sampling because after the dry season by the end of the harvest time, all the applied fertilizers are completely leached out of the soil profile.

In this study area there is not any second cultivation, therefore, all the nitrogen is likely to be washed away and leached into the groundwater. Water samples at different depths were collected and analyzed for nitrate and nitrite concentrations for three continuous years from 2011 to 2014. The sampling was performed 20 times at 0–30 and 30–60 cm depth. The sampling instrument was consisted of one oger which was a hollow tube with sharp head.

The analysis of water samples was done using a DR2000 device in the health department of Babol medical center. In 82 % of samples nitrate Concentration exceeded the USEPA standard, however, nitrite concentration in all samples fell within the standard range. Nitrate concentration in all samples of rice field was higher than the standard limit while no sample in citrus cultivation area exceeded the standard limit. The mean nitrate and nitrite concentration in all samples were 20.3 and 0.12 mg/l, respectively. The laboratory measured data were soil saturation percent, electrical conductivity, acidity, organic matter percent, carbon percent and the total available nitrogen at each soil sampling. Huang et al. (2011) showed that groundwater runoff modulus in previous system is not important as input data for neural networks. Therefore, in this study, this parameter was not measured. Table 2 shows the average, maximum and minimum of the soil and groundwater measured parameters. Numbers of wells in each range of concentration are shown in Table 3. The sample analyses showed nitrate concentration is higher than USEPA nitrate recommendation in drinking water and it justifies the importance of regional groundwater studies.

Table 2 Measured soil and water parameters in Babol

Parameters	Min	Max	Average
Saturation percentage in soil (percent)	39	92	66.4
EC × 10^{-3} in soil	0.24	3.17	1.23
pH in soil	6.06	8.19	7.48
Organic matter in soil (percent)	0.75	7.52	2.95
Total nitrogen in soil (percent)	0.015	0.33	0.152
Organic carbon in soil (percent)	0.53	3.835	1.67
NO2 in ground water (mg/l)	0.03	0.31	0.12
NO3 in ground water (mg/l)	4.3	45.5	20.88

Artificial neural network modeling

At first step, the Pearson formula was used to determine the main measures for neural network model as input. Next, two kinds of neural network (BPNN and Radial base) was developed to be used for prediction of nitrate in regional groundwater. Correlation analysis of all influential variables associated with the groundwater nitrate concentration was performed using the Pearson formula.

The results are shown in Table 3. The analyses demonstrated that variables such as soil nitrogen content, soil carbon content, soil organic matter content and the nitrite concentration in water are the most influential factors affecting the groundwater NO_3-N concentration, significant at the 0.01 level in a two-tailed test.

According to Table 4 nitrite in ground water (X), soil organic matter content (Y), soil nitrogen content (Z) and pH (T) were chosen as input layers for artificial neural network, and groundwater NO_3-N concentration (R) was the output layer. Then the ANN model with functional relationship of R = f (X, Y, Z, T) was established.

ANNs are analytical techniques, capable of acquiring the knowledge and modeling the complex environmental processes. For predictive purposes, such modeling is done using the observed data for storing the knowledge of underlying process, and thus synthesize it to be applied to new observations (test phase). In order to optimally predict (find a best fit for) the sample data, during the training phase in which the knowledge of an environment is acquired from the observed data; an iterative learning algorithm is applied to the number of inputs (variables) to find the optimal adjustment of the network connection weights (Sahoo et al. 2005).

Two well-known ANN models, the feed-forward BP and the radial basis function (RBF), were employed as preliminary exploratory models to investigate their efficiency for the purpose of nitrate detection in ground water. The MATLAB toolbox was used to create BP and RBF type neural networks for this study.

Table 3 Number of wells in each concentration range and percentage

Concentration range nitrate (mg/l)	Number of samples in the range	Percentage of samples in the range
0–5	4	4.30
5–10	13	13.98
10–15	15	16.13
15–20	19	20.43
20–30	26	27.96
30–40	7	7.53
40–50	9	9.68

Table 4 Pearson correlation results

Parameters	Correlation with groundwater NO_3-N concentration
NO_2 in ground water (mg/l)	0.759
Saturation percentage	−0.037
EC × 10^3	0.036
pH	−0.115
Organic matter	0.086
Organic carbon	0.075
Total nitrogen	0.156

Table 5 Suggested rule for number of neuron layer in BPNN networks

References	Equation	Number of hidden layer
Patuwo et al. (1993)	2 I + 1	9
Wang (1994)	2 I/3	3
Piramuthu et al. (1994)	0.5 (I + O)	2
Lenard et al. (1995)	0.75 I	3
Kanellopoulos and Wilkinson (1997)	2 I	8
Kanellopoulos and Wilkinson (1997)	3 I	12

Back propagation neural network

In this study, the back-propagation training algorithm is applied which is also the most widely used neural network method. After the training phase, in which the internal weights are adjusted, the classifying process begins as the second stage in application of neural networks for multi-source classification. Basically, the back-propagation algorithm trains the network until the minimum target error between the desired and actual output values is reached or the number of iterations exceeds the preset maximum number. When this criterion is met, the network is sufficiently trained and may be used as a feed-forward classifier to obtain a classification of the entire dataset (Huang et al. 2011). Table 5 illustrates practical research recommendations about the number of neurons as the most important feature of BPNN. Ultimately, the distribution pattern of groundwater nitrate concentration can be obtained after appropriate training, calibration and validation. The back-propagation algorithm determines the optimal weighting of the features by iterative modification of the hidden nodes and the learning rate while calculating the relative weights between the input and the hidden layers, and between the hidden and the output layer (Choi et al. 2010). The feed forward network modeling and analysis were performed using the MATLAB software. The term ''feed-forward'' denotes that the data presented to the input layer are propagated in a forward direction to the next layer by the interconnections between the neurons.

An optimal choice of network parameters such as the number of hidden layers and nodes within a layer, needed for a particular classification problem is not easy to achieve. Table 5 presents some recommendations and heuristic rules for choosing the number of neurons suggested by other studies. In this table, I denotes the number of input layer and O is the number of output layer. In the present study, four input parameters including nitrite concentration, soil organic matter content, soil nitrogen content and pH are employed where the only output is nitrate in groundwater. Therefore, the initial number of hidden layers is chose between 1 and 12 while also 15 was selected as an out of range boundary value.

The BPNN architectures were specified selectively to ensure the minimum difference between the measured data and the predicted data. The mean square error (MSE), used as the target error goal, is defined as:

$$MSE = \frac{\sum_{i=1}^{n} (T_i - R_i)^2}{n} \quad (1)$$

where n is number of input samples, T_i and R_i are the target and observed NO_3-N concentration in groundwater, respectively. Training stops when any of these conditions occur: (1) the maximum number of epochs (repetitions) is reached, (2) performance has been minimized to the target error goal (MSE in this case), and (3) the performance gradient falls below the minimum gradient (Principe et al. 1999). Therefore, if the minimum performance gradient falls below 10^{-10} the termination of the training process is justified as further training would not provide any performance improvement (Hagan et al. 1996).

According to previous studies (Maier and Dandy 1998; Ray and Klindworth 2000), a tangent sigmoid transfer (between −1 and 1) function is used for hidden layers and a linear transfer (between $-\infty$ and ∞) function was used for output layer. The back-propagation algorithm adjusts the network weights to minimize the error between the predicted and actual outputs. This algorithm propagated the error backwards while iteratively adjusted the weights. The maximum numbers of epochs, target error goal 'MSE', and the minimum performance gradient were set to 1000, 0.01, and 10^{-5}, respectively. Therefore, if the gradient value falls below 10^{-5} the training process terminates or else the training process will continue till the end of 1000 epochs. The idea is to let the system train until the point of diminishing returns (MSE = 0.01). All the iterations met the 0.01 root mean square error goal or the training process will continue till the end of 1000 epochs. It should be mentioned that the toolbox of MATLAB software was used to create BPNN. The input data were normalized to the range of 0–1, while 70 %of the data used as training, 25 % for test and 5 % as validation sets.

Radial basis function neural networks (RBFNN)

Radial basis function neural networks (RBFNN) advantages over traditional multilayer perceptron models such as faster convergence, smaller extrapolation errors, and higher reliability makes them exceedingly promising for engineering applications (Moradkhani et al. 2004). Like the back-propagation network, the RBF neural network has a feed-forward architecture that is very similar to a multilayer perceptron network (MLP). It consists of three layers: (1) one input layer, (2) only one hidden layer that obviously reduce the computation time, and (3) one output layer as shown in (Fig. 2), in which numbers of neurons are N, M, L, respectively. The self-organized characteristic of the RBF structure allows for adaptive determination of hidden neurons during the training phase (Zhang and Kushwaha 1999).

An input pattern enters the input layer and the neurons in the input layer just propagate input features to the next layer, whereas output from input layer is same as the input pattern. Number of nodes in the input layer is equal to the dimension of input vector p as:

$$P = [p_1 p_2 \cdots p_n]^T, \tag{2}$$

N is number of input nodes, and Pi is the output layer

The hidden layer consists of locally tuned units each of which has radial basis function acting like a hidden node. Each node in this layer must have the following features as: (a) A center vector Cj in the input space while M is the number of center vectors. (b) A distance measure to determine how far an input pattern Pi is from elements of center vector C_{ji}.We have used Euclidean distance norm to

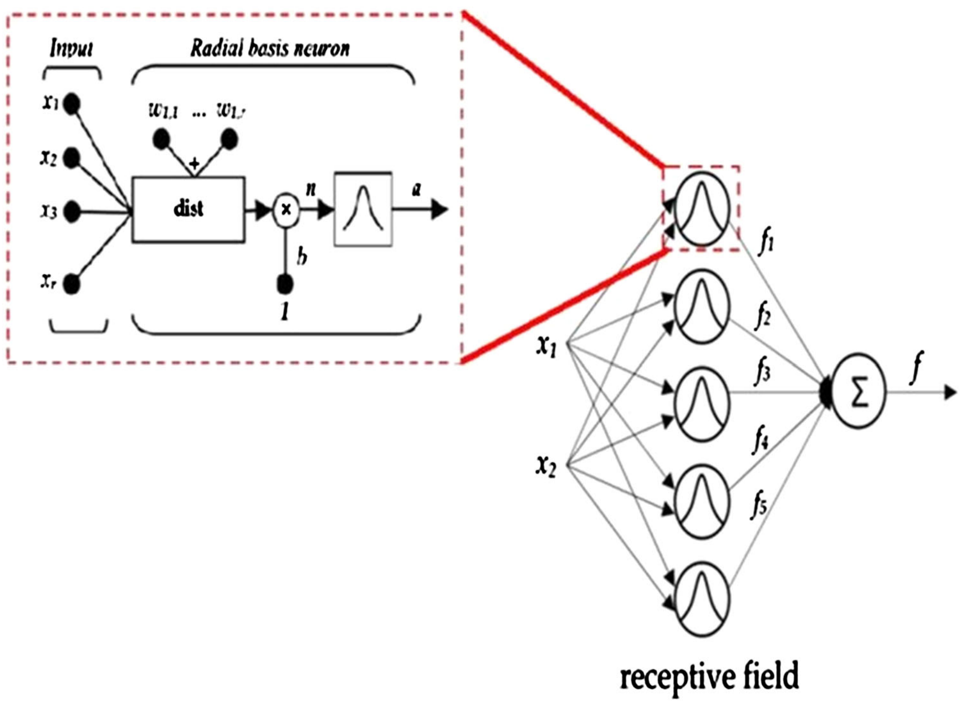

Fig. 2 Radial basis structure

Table 6 Performance of different BPNN structures

Number of node	R train	R test	MSE (mg/l) in train	MSE (mg/l) in test
2	0.68	0.75	0.83	0.47
3	0.64	0.88	0.80	1.12
5	0.86	0.66	0.35	0.72
8	0.81	0.82	0.42	1.64
9	0.81	0.58	0.53	1.40
12	0.94	0.77	0.13	0.88
15	0.71	0.87	1.03	1.21

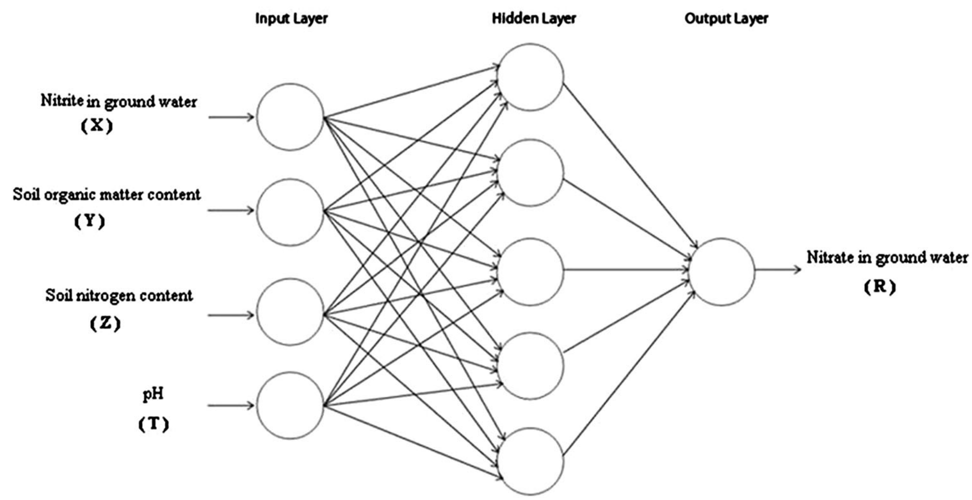

Fig. 3 Best BPNN network structure

measure distance between input vector P and node j of hide-layer.

$$\text{Euclidean distance edj} = \|P - Cj\| = \sqrt{\sum_{i=1}^{N} (P_i - C_{ji})^2}; \quad i = 1, 2, \ldots, N \tag{3}$$

(c) A transfer function φ which transfers Euclidean distance to give output for each node. (In this study we consider a Gaussian function).

$$\varphi_j(P) = \exp\left(-\frac{1}{2\sigma_j^2}\left\|P - Cj^2\right\|\right); \quad j = 1, 2, \ldots, M \tag{4}$$

where σ is the spread parameter that represents the width of the radial basis function (Sahoo et al. 2005). There are weight factor w_{kj} (k = 1 to L, j = 1 to M) between kth nodes of output layer and jth nodes of hidden layer. 'L' is the dimension of output vector. output from output layer transferred through a transfer function like log sigmoid or tan sigmoid. The kth network output can be calculated as:

$$\text{Output}_k = f\left(\sum_{k=1}^{L} w_{kj} \times \text{Output}_j\right); \quad k = 1,2, \ldots, L \tag{5}$$

Calculation and modeling of ANNS, experiment was conducted in the MATLAB 2008 environment. It has been tried to minimize the network error in the training process. Then, the results are compared with measured values using MSE (mean square error) on training procedure.

Results and discussion

The retrieval results by BPNN

The advantage of using neural networks is the ability to properly describe nonlinear and interacting relationships within a regional crop–soil–groundwater system (Paola and Schowengerdt 1995). In the developed model, the routine

Table 7 The final trained weights and biases in the control run with the optimum parameters

The weights in the input-hidden layers				
W1,1 = 1.468	W2,1 = −0.0650	W3,1 = −0.2332	W4,1 = −1.4408	
W1,2 = −0.814	W2,2 = −0.0829	W3,2 = −1.8868	W4,2 = −0.8036	
W1,3 = 0.191	W2,3 = −2.0920	W3,3 = 0.9399	W4,3 = 1.3919	
W1,4 = 1.028	W2,4 = 0.9717	W3,4 = −1.3459	W4,4 = −1.0354	
W1,5 = 0.228	W2,5 = −0.3528	W3,5 = 0.5727	W4,5 = 1.9210	
The weights in the hidden-output layers				
W1,1 = −0.2889	W2,1 = −0.5374	W3,1 = 0.6061	W4,1 = 1.0599	W5,1 = −0.3846
The biases in the hidden layer				
b1 = −2.1094	b1 = 0.4812	b1 = 0.0427	b1 = 0.7710	b1 = 2.5049
The biases in the output layer				
b2 = −0.121				

data of soil characteristics, groundwater monitoring, field fertilizer usage and management measures can easily be used as input data without any preliminary specialized testing and time consuming parameter identification. A very important feature of neural networks is their adaptive nature which enables them to quickly represent the updated system characteristics by continuous adaption to the changing environmental factors or human activities. The model verification results confirmed the BPNN strong learning ability, robustness, and high predictive accuracy for nonlinear systems. Table 6 shows how the optimum number of nodes in hidden layer of back propagation neural network was estimated.

The model with two neurons in hidden layer showed the least square error in the test stage. Although it is found to have a low correlation coefficient, at the same time the number of false values in training stage was significantly more than testing stage. Therefore, this neurons architecture was recognized as unsuitable. Comparative analysis of the neurons system behavior indicated that the best result would occur with five neurons in hidden layer. Consequently, the 4-5-1 structure is adopted for the BPNN as it is shown in Fig. 3.

The layers weights acquired by the training phase were calculated in reverse to represent the contribution or importance of each factor.

For development of the current network 38 vectors selected for training from a total sample of 50. Twelve vectors used for test set. At the third step, we train the network to get the statistical analyses. The physical meaning of parameters is equivalent to the grid structure, serves as testing and the input of identifying of new samples. The fourth step was statistical analyses of output parameters. The 'newrb' function available in the commercial MATLAB toolbox was used to create a radial basis neural network. Initially there is no radial basis neuron. It iteratively creates one radial basis neuron at a time and adds neuron to the network until either the sum squared error falls beneath an error goal (MSE) or the maximum number of neurons is reached. The values of error goal (MSE) in MATLAB toolbox were selected equal to (0.01, 0.02, 0.03, or 0.04), and spread were selected equal to (0.5 or 0.8 or 1). The selected transfer function in output layer is 'pureline' function. The results of the modeling are shown in Table 7.

Radial basis result

The entering data for BPNN network normalized in 0–1 distance and 25 % of data has been selected as test and 75 % has been selected as training sets. It is necessary to mention that this data are the same random data as BPNN network test data and during training phase was found that Training Performance is equal to one. This infers that our predictive model is trained well. Since the neurons in the hidden layer of RBF network respond to inputs in the neighborhood of their centers, they develop a composition of localized receptive fields.

Table 8 The calculated performance indices for radial basis function neural network models

Case RBF (spread, goal)	Training performance R	Validation Performance	
		MSE (mg/l)	R
RBF (0.5, 0.01)	1.0	4.78	−0.192
RBF (0.5, 0.02)	1.0	1.23	0.31
RBF (0.5, 0.03)	1.0	0.50	0.85
RBF (0.5, 0.04)	1.0	1.09	0.37
RBF (0.8, 0.01)	1.0	5.60	−0.074
RBF (0.8, 0.02)	1.0	10.46	0.48
RBF (0.8, 0.03)	1.0	0.65	0.77
RBF (0.8, 0.04)	1.0	0.65	0.77
RBF (1, 0.01)	1.0	8.08	−0.28
RBF (1, 0.02)	1.0	0.71	0.69
RBF (1, 0.03)	1.0	0.69	0.7
RBF (1, 0.04)	1.0	0.69	0.7

A sensitivity analysis was carried out to ensure the optimum spread values are chosen to minimize model prediction error. It is proved that the RBF with a spread of 0.5 can achieve better results than RBF with spread 1.0 (default value of MATLAB toolbox) or higher spreads. Also it was found that lower spread values (< 0.5) may not lead to any performance improvement.

Therefore, a good choice of the spread value in a typical RBF network is a determining factor for its successful application in achieving the most accurate simulation results. According to Table 8 best Radial Basis network which can predict the nitrate in groundwater have their spread and error goal as 0.5 and 0.03, respectively. Thus, the network weights were determined, as measures of each parameter effective contribution and influence on the system. The final trained weights and biases of a randomly run with the optimum parameters are shown in Table 9.

Conclusions

Two types of neural networks; back-propagation neural network, and a radial basis function (RBF) were tested for prediction of nitrate in groundwater from analyzed groundwater N concentration, soil organic matter content, soil nitrogen content and pH as input data. Since sample collection, analysis, and re-sampling are expensive, only 50 samples from 50 wells were used for analyses in this study. Among the various structures of BPNN and RBF networks employed for this study, BPNN with five neurons in hidden

Table 9 Trained weights and biases in best radial basis training phase

The weights in the input-hidden layers			
W1,1 = 0.75	W2,1 = 0.3454	W3,1 = 0.4009	W4,1 = 0.5714
W1,2 = 0.8571	W2,2 = 0.09980	W3,2 = 0	W4,2 = 0.1428
W1,3 = 0.6071	W2,3 = 0.5547	W3,3 = 0.5930	W4,3 = 0.7460
The weights in the hidden-output layers			
$W_{1,1} = -0.0578$	$W_{2,1} = 0.9158$	$W_{3,1} = 0.7813$	
The biases in the hidden layer			
$b_1 = 1.6651$	$b_1 = 1.6651$	$b_1 = 1.6651$	
The biases in the output layer			
$b_2 = -0.0622$			

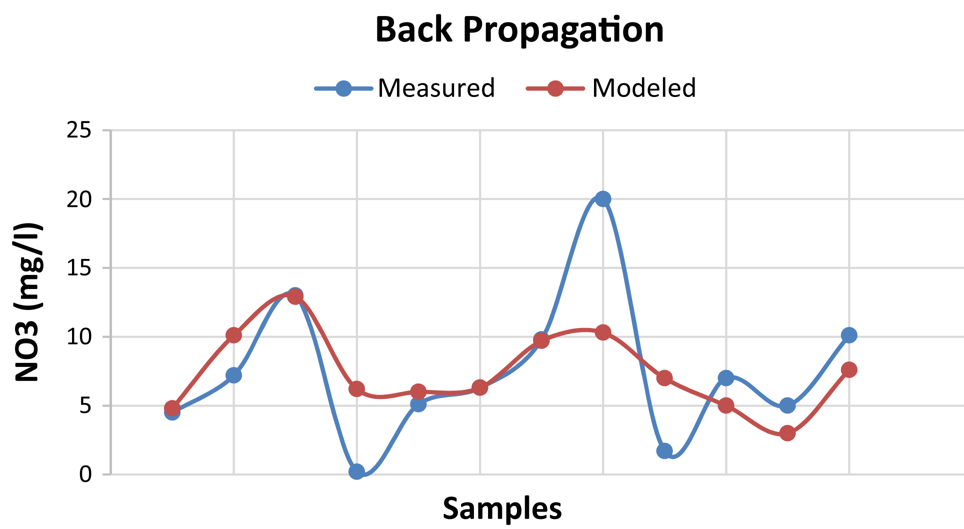

Fig. 4 Comparison of the measured and simulated NO_3 in the ground water, back propagation neural network

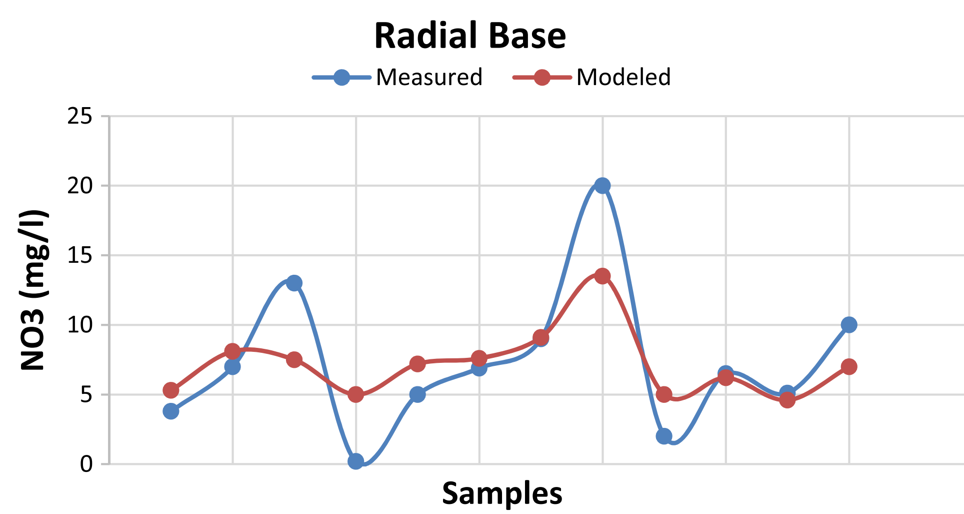

Fig. 5 Comparison of the measured and simulated NO_3 in the ground water, radial base neural network

layer was found to be superior to other structures. The prediction ability of the RBF neural network was found to be marginally better than BPNN. Figures 4 and 5 show the comparison between BPNN and RBF in process of validation step. It shows RBF could differentiate the trend slightly more accurate than PBNN. Moreover, weights and biases are illustrated in Tables 7 and 9 to determine values of each parameter in different layers. ANN models can predict nitrate contamination in groundwater with acceptable accuracy. However, the radial base model had a marginally better performance compared to the back-propagation by 30 %.

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