Groundwater quality modeling using neuro-particle swarm optimization and neuro-differential evolution techniques

Ozgur Kisi, Ali Keshavarzi, Jalal Shiri, Mohammad Zounemat-Kermani and El-Sayed Ewis Omran

ABSTRACT

Recently, the capabilities of artificial neural networks (ANNs) in simulating dynamic systems have been proven. However, the common training algorithms of ANNs (e.g., back-propagation and gradient algorithms) are featured with specific drawbacks in terms of slow convergence and probable entrapment in local minima. Alternatively, novel training techniques, e.g., particle swarm optimization (PSO) and differential evolution (DE) algorithms might be employed for conquering these shortcomings. In this paper, ANN-PSO and ANN-DE models were applied for modeling groundwater qualitative parameters, i.e., SO_4 and sodium adsorption ratio (SAR). Three statistical parameters including root mean square error (RMSE), mean absolute error (MAE), and the coefficient of determination (R^2) were used for assessing the models' capabilities. The results showed that the ANN-DE presents more accurate results than ANN-PSO in modeling SAR and electrical conductivity (EC).

Key words | artificial neural network, differential evolution, groundwater quality, particle swarm optimization

Ozgur Kisi
Center for Interdisciplinary Research,
International Black Sea University,
Tbilisi,
Georgia

Ali Keshavarzi
Laboratory of Remote Sensing and GIS,
Department of Soil Science,
University of Tehran,
Karaj 31587-77871, Iran

Jalal Shiri (corresponding author)
Water Engineering Department, Faculty of Agriculture,
University of Tabriz,
Tabriz, Iran
E-mail: *j_shiri2005@yahoo.com*

Mohammad Zounemat-Kermani
Department of Water Engineering,
Shahid Bahonar University of Kerman,
Kerman, Iran

El-Sayed Ewis Omran
Soil and Water Department, Faculty of Agriculture,
Suez Canal University,
Ismailia, Egypt

INTRODUCTION

Groundwater is one of the major sources of water supply of domestic as well as agricultural activities. Modeling groundwater quality is needed to develop better strategies for water resources planning and management (Liu *et al.* 2009; Najah *et al.* 2014). Traditional water resources management approaches considered surface water and groundwater systems as two separate entities. However, the recent developments in land and water resources analysis have demonstrated that these systems could affect each other, from both qualitative and quantitative points of view. Nonetheless, groundwater contamination, either by anthropogenic activities, or by inherent aquifer material composition, reduces groundwater supply capacity or restricts its exploitation.

Meanwhile, agricultural activities, which might include the uncontrolled use of fertilizers and pesticides, influence and cause the deterioration of groundwater quality, although variations in groundwater quality can be influenced by geological formations and anthropogenic activities, too (Yesilnacar *et al.* 2008). Variation of groundwater quality is a component of physical and chemical parameters that are enormously impacted by geological formations and anthropogenic activities (Almasri & Kaluarachchi 2005; Subramani *et al.* 2005; Yesilnacar & Sahinkaya 2012).

Electrical conductivity (EC) illustrates the capacity of a substance or solution to conduct the electricity current. EC is a good predictor for obtaining total dissolved solids

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(TDS), which is a measure of all inorganic and organic substances (WHO 1984). Having the values of Na^+, Ca^{2+}, and Mg^{2+}, sodium adsorption ratio (SAR) can be calculated as (Devadas et al. 2007):

$$SAR = \frac{[Na^+]}{(([Ca^{2+}] + [Mg^{2+}])/2)^{1/2}} \tag{1}$$

where the ion concentrations are in meq/L.

Nevertheless, the hardness of groundwater might be calculated as:

$$\text{Hardness}\left(\frac{as\, mg\, CaCO_3}{L}\right) = \frac{(Ca^{2+} + Mg^{2+})meq}{L} \times 50 \tag{2}$$

SAR, which is determined by the concentrations of solids dissolved in the water, is a significant parameter for analyzing the suitability of irrigation water. Higher SAR values (high Na^+ and low Ca^{2+} and Mg^{2+} magnitudes) may cause the dispersion of clay particles and destroy the soil structure (Yesilnacar & Sahinkaya 2012). Nevertheless, groundwater sulfate might be provided to the point and non-point sources. The maximum permissible and allowable concentrations of sulfate in drinking water are 200 and 400 mg/l, respectively (WHO 1984). High sulfate concentrations affect the water taste. Therefore, groundwater SAR and sulfate simulation are important tasks in groundwater resources management and planning.

The traditional groundwater quality analysis approach is mainly based on mathematical modeling, e.g., time series analysis, probability statistics, etc., which usually assume a linear relationship between the dependent and independent variables, thus the model's overall accuracy is not high (Luo et al. 2003). Owing to the existing difficulties in simulating groundwater quality (Omran 2012), novel computational approaches are required.

As an alternative to the traditional statistical approaches, artificial intelligence techniques might be used to solve this problem. Among others, artificial neural networks (ANNs) have been widely applied in numerous disciplines, e.g., qualitative/quantitative groundwater modeling (Cheng et al. 2005; Liu & Chung 2014). Yesilnacar et al. (2008) predicted groundwater nitrate concentration in Harran Plain in Turkey using ANNs. Yesilnacar & Sahinkaya (2012) developed an ANN model for predicting groundwater sulfate (SO_4) and SAR concentration. Kuo et al. (2004) utilized back-propagation ANN to predict the variations of groundwater quality (in terms of seawater salinization and arsenic pollutant factors) in Taiwan. Khaki et al. (2015) evaluated the potential of adaptive neuro-fuzzy inference system (ANFIS) and ANN to simulate TDS and electrical conductivity (EC) levels.

Despite ANNs' capability in modeling nonlinear systems, establishing these models with conventional training algorithms may produce non-optimum outcomes because of limitations for adapting the best synaptic weights. Alternatively, ANN models might be integrated with some evolutionary algorithms (EAs), e.g., differential evolution (DE) and particle swarm optimization (PSO) to optimize the models' structures.

DE is a meta-heuristic population-based algorithm, which can be used for multidimensional real-valued functions. The PSO algorithm evolves a population of particle individuals through an iterative process to find the optimized solution. Unlike most EAs, PSO has low computational costs and its implementation is straightforward. Each potential solution in PSO is represented by a particle, flies in a multidimensional search space with a velocity dynamically adjusted by the particle's own former information and the experience of the other particles. Numerous applications of PSO have been reported in solving real-world optimization problems (e.g., Liu et al. 2007; Melin et al. 2013; Selakov et al. 2014).

Karterakis et al. (2007) applied DE for the solution of coastal subsurface water management problems. Gaur et al. (2011) applied an analytic element method coupled with PSO for groundwater management and reported that the developed model is efficient in identifying the optimal location and discharge of the pumping wells. Sudheer & Shashi (2012) developed a PSO trained ANN for aquifer parameter estimation. Gaur et al. (2013) applied ANN and PSO for management of groundwater and reported that the ANN-PSO model is capable of identifying the optimal location of wells efficiently. Chiu (2014) applied DE for parameter structure identification in groundwater modeling. Elci & Ayvaz (2014) applied a DE algorithm-based optimization for the site selection of groundwater production wells. Based on a review study, Ketabchi & Ataie-Ashtiani (2015) investigated the literature associated with the application of evolutionary algorithms (e.g., PSO and DE algorithms) in coastal groundwater management problems. Overall, they concluded that the PSO algorithm is among the superior EAs.

In the present study, the capability of PSO and DE algorithms were evaluated in modeling groundwater quality parameters (i.e., SO_4 and SAR).

MATERIALS AND METHODS

Site description

This study was conducted in Neyshabur plain, Iran, located between 35°41′ (°N) and 58°20′ (°E) (Figure 1). The average altitude of the region is 1,500 m above mean sea level. Mean annual precipitation and temperature values are 233.7 mm and 14.5 °C, respectively (Mansouri Daneshvar *et al.* 2013).

Groundwater sampling and measurement

Monthly groundwater records were collected from 60 observational wells during a 16-year period (1997–2013).

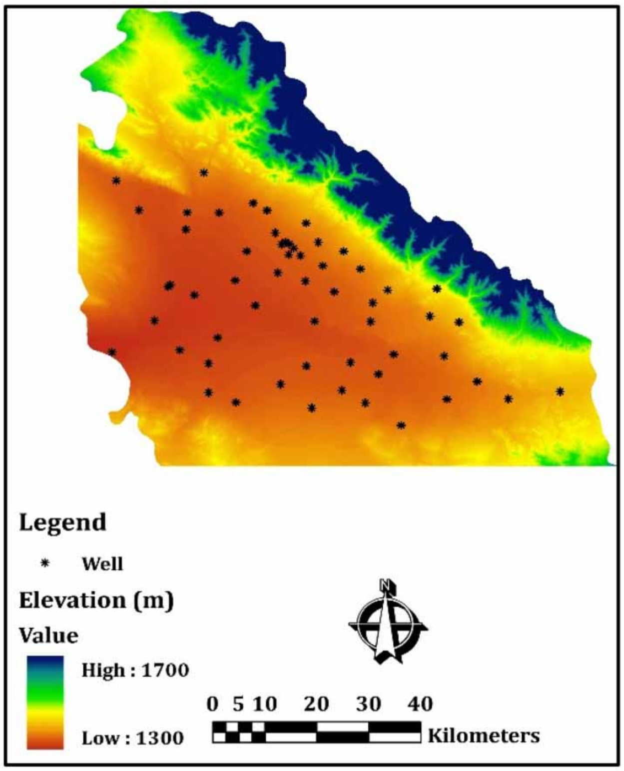

Figure 1 | Location of the study area and sampling wells.

Geographical coordinates and elevation of each sampling location was recorded using a handheld global positioning system (GPS). A few locations were also cross-checked with a differential GPS. Collected samples were analyzed in the laboratory to measure the concentration of the qualitative parameters using the existing standard procedures (Table 1).

In this study, groundwater qualitative parameters, i.e., SO_4 and SAR were modeled using two different evolutionary neural networks, namely, ANN-PSO and ANN-DE. Calcium, magnesium, sodium, hardness, electrical conductivity, TDS, pH, bicarbonate, and chloride parameters were used as input variables to estimate the SO_4 and SAR. Table 2 sums up the statistical parameters of the applied data. Variability class of the coefficient of variation (CV) was obtained based on the criterion presented by Wilding (1983). Based on this criterion, the CV values less than 15% denote the low variability class, while the CV values higher than 35% stand for the high variability class. The CV values between 15% and 35% correspond to the medium variability class. Considering the results presented in Table 1, high variations were observed in groundwater qualitative parameters (from 41.92% to 123.98%), except pH, which shows low variability with a CV value of 4.72%. For developing the applied models, 50% of data (1,200 patterns) were used for training, while the remaining

Table 1 | Utilized methods for hydro-chemical parameters identification in the present study

Parameter	Method
Electrical conductivity (μS/cm)	Conductivity bridge (Richards 1954)
pH	pH meter (Thomas 1996)
Sodium (mg/L)	Flame photometric (Osborn & Johns 1951)
Calcium (mg/L)	EDTA titration (Richards 1954)
Magnesium (mg/L)	EDTA titration (Richards 1954)
Bicarbonate (mg/L)	Acid titration (Hesse 1971)
Chloride (mg/L)	Mohr's titration (Hesse 1971)
Hardness (mg $CaCO_3$/L)	EDTA titration (Richards 1954)
Total dissolved solids (ppm or mg/L)	Water quality analyzer (APHA 1995)

EDTA, ethylenediaminetetraacetic acid.

Table 2 | The range of measured values of the groundwater quality properties

Parameter	Unit	Min	Max	Mean	Std	CV
EC	μS/cm	4.40	35,200.00	2,946.69	3,102.26	105.28
pH	–	6.30	9.50	8.00	0.37	4.72
Sodium	mg/L	0.00	127.30	18.52	18.89	101.99
Calcium	mg/L	0.00	40.60	4.75	5.26	110.58
Magnesium	mg/L	0.00	44.80	5.051	4.43	87.79
Bicarbonate	mg/L	0.00	11.00	2.93	1.23	41.92
Chloride	mg/L	0.00	142.50	17.60	21.83	123.98
TH	mg $CaCO_3$/L	0.00	3,625.00	490.47	448.69	91.48
TDS	ppm or mg/L	2.77	2,2176.00	1856.42	1954.42	105.26
SO_4	mg/L	0.00	50.00	8.49	7.64	90.01
SAR	–	0.00	37.89	8.06	6.77	84.03

Std: standard deviation, CV: coefficient of variation (%).

25% and 25% (600 and 600 patterns) was used for validating and testing the models, respectively.

Applied algorithms

Artificial neural networks

ANNs are interconnected groups of artificial neurons (processors) designed for information processing through a computational model. They are generally utilized to simulate the output vectors according to the given input vectors, especially in dynamic systems where the interrelationships between the input-target parameters are non-linear (Omkar & Senthilnath 2011; Balouchi *et al.* 2015). In an ANN structure, input and output vectors are placed as the first and last layers. Among these layers, hidden layer(s) with several neurons are considered. In this study, a neural network with one hidden layer was established and the number of neurons in the hidden layer was determined iteratively. The schematic diagram of the applied feed-forward ANN is shown in Figure 2.

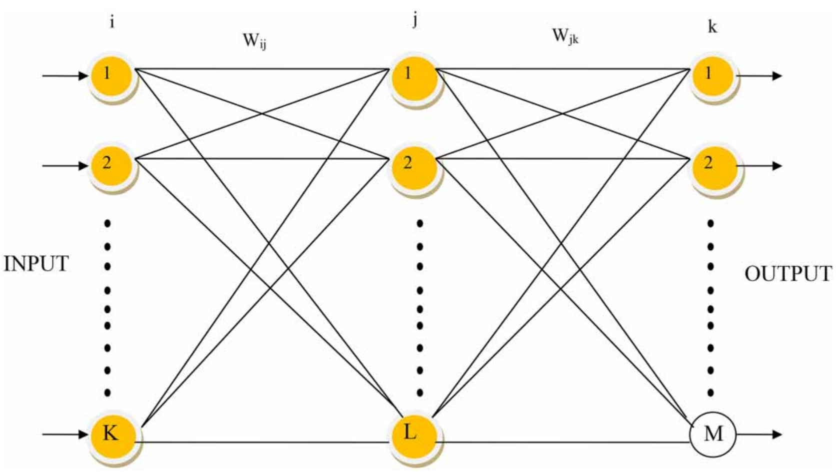

Figure 2 | A three-layer ANN architecture.

Particle swarm optimization

PSO is an evolutionary computation algorithm, based on iterative optimization (Kennedy & Eberhart 1955). PSO consists of a group of particles (individuals) which refine their knowledge of the search space. Each particle has two main characteristics of position and velocity. In the PSO, the iterative method is used to reach the optimal solution according to the fitness values of each particle, which is determined by optimization function. Each particle adjusts its trajectory by tracking two pieces of information: (1) the best visited position (Pbest) and (2) the global extremum attained by species (Gbest) (Assareh *et al.* 2010). At each generation (iteration) step, each particle is accelerated toward the previous Pbest and the Gbest position of the particle. A new velocity magnitude is calculated for each particle based on its current velocity and its distance from its previous Pbest and Gbest. The updated velocity magnitude is then utilized to calculate the next position of the particle through the search space. The iterative process is continued a set number of times, or until achieving a minimum error.

In PSO, a population of particles or proposed solutions evolves in each iteration, moving towards the optimal solution of the problem. A new population is obtained shifting the positions of the previous one for each iteration. In its movement, each individual is influenced by its neighbors' and its own trajectory. The parameters, or possible set of solutions, are contained in a vector x_i, which is called a 'particle' of the swarm and represents its position in the search space of possible solutions. The particle dimension is the number of parameters. The particle position x_i^0 and its velocity v_i^0 are randomly obtained. The value of the fitness function is then calculated for each particle and the velocities and positions are updated taking into account these values. The algorithm updates the positions and the velocities of the particles following the equation:

$$v_i^{k+1} = \omega v_i^k + \varphi_1(g^k + x_i^k) + \varphi_2(I_i^k + x_i^k) \quad (3)$$

The velocity of each particle, i, at iteration k, depends on three components:

- the previous step velocity term, v_i^k affected by the constant inertia weight, ω;
- the cognitive learning term, which is the difference between the particle's best position so far found (called I_i^k, local best) and the particle current position x_i^k;
- the social learning term, which is the difference between the global best position found thus far in the entire swarm (called g^k, global best) and the particle's current position x_i^k.

These two last components are affected by $\varphi_1 = c_1 r_1$ and $\varphi_2 = c_2 r_2$ where r_1 and r_2 are random numbers distributed uniformly in the interval [0,1] and c_1 and c_2 are constants. The particles of the swarm make up a cloud that covers the whole search space in the initial iteration and gradually contracts its size as iterations advance, performing the exploration. Thus, in the initial stages the algorithm performs an exploration searching for plausible zones and in the last iterations the best solution is improved. The PSO implementation of the algorithm has been refined over the years and many variants created. In this paper, the Standard 2011 PSO has been used. It contemplates some improvements in the implementation and the PSO parameters are set to the values:

$$\omega = \frac{1}{2\ln 2} \text{ and } c_1 = c_2 = 0.5 + \ln 2 \quad (4)$$

The swarm topology defines how particles are connected between them to interchange information with the global best. In the actual Standard PSO each particle informs only K particles, usually three, randomly chosen.

Differential evolution

DE is a population-based stochastic search technique for solving continuous optimization problems. DE algorithm comprises three major operators, namely, mutation, crossover, and selection. Mutation is the simplest genetic operator. It randomly flips bits in a binary string genome from 0 to 1 or from 1 to 0. This operator improves the algorithm by introducing new solutions that do not exist in the population. After initialization, mutation operation is employed with respect to each target individual $x_i(t)$. Thereafter, a mutant vector $V_i(t)$ is determined by the current population by the following equation (Storn 1996):

$$V_i(t) = x_{i1}(t) + F(x_{i2}(t) - x_{i3}(t)) \quad (5)$$

where i_1, i_2 and i_3 are randomly chosen indices selected within the range {1, 2,…,NP}. After the mutation, crossover operation, which is the process of varying DNA of chromosomes by exchanging some of their sections, is applied. It applies to each $x_{ij}(t)$ (pair of the target vector) and its related mutant vector $v_{ij}(t)$ to generate $u_{ij}(t)$ as an offspring vector can be considered as:

$$u_{ij}(t) = \begin{cases} v_{ij}(t) & \text{if} \quad U(0,1) < P_r \quad \text{or} \quad j = r, \\ x_{ij}(t) & \text{otherwise} \end{cases} \tag{6}$$

Even when $P_r = 0$, at least one of the parameters of the offspring will differ from the parent (forced by the condition $j = r$). A number of individuals from the existing generation are selected to breed a new generation. The selection is typically based on fitness. Thus, the fitter an individual is, the more likely it is to be selected. A weak individual still has a chance to be selected, and this helps to keep the diversity of the population high. The trial vector $U_i(t) = \{u_{i1}(t), u_{i2}(t), \ldots, u_{iD}(t)\}$ is going to be selected as a member of the population comprising the next generation after being compared to the corresponding target vector $x_i(t)$. The selection operator for the next target vector is as below:

$$x_i(t+1) = \begin{cases} u_i(t), & f(u_i(t)) < f(x_i(t)), \\ x_i(t) & \text{otherwise} \end{cases} \tag{7}$$

These steps are repeated until a pre-specified stopping criterion is satisfied.

The conventional ANN models utilize gradient-based algorithms (GBAs) (e.g., back-propagation) for identifying the weights. For the GBAs, in the calibration (training) period, it is very easy to get trapped in a local minima (Kumar *et al.* 2002; Sudheer *et al.* 2003). The evolutionary algorithms (e.g., PSO, DE) are more robust than the existing direct search methods (e.g., GBAs) because they combine the stochastic and direct search. Evolutionary algorithms (EA) provide the global optimum without being trapped in local optima as in the GBAs (Mantoglou *et al.* 2004; Karterakis *et al.* 2007).

Goodness-of-fit of the model

The ANN-PSO and ANN-DE models were evaluated according to three goodness-of-fit measures, namely, the root mean square error (*RMSE*), the mean absolute error (*MAE*), and the coefficient of determination (R^2), expressions of which are as follows:

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(WQ_{i,o} - WQ_{i,e})^2} \tag{8}$$

$$MAE = \frac{1}{N}\sum_{i=1}^{N}|WQ_{i,o} - WQ_{i,e}| \tag{9}$$

$$R^2 = \left(\frac{\sum_{i=1}^{n}(WQ_{io} - \text{mean}WQ_o)(WQ_{ie} - \text{mean}WQ_e)}{\sqrt{\sum_{i=1}^{n}(WQ_{io} - \text{mean}WQ_o)^2 \sum_{i=1}^{n}((WQ_{ie} - \text{mean}WQ_e))^2}}\right)^2 \tag{10}$$

where N is the number of data, $WQ_{i,o}$ denotes the observed water qualitative parameters (SO_4 or SAR) value, and $WQ_{i,e}$ denotes the corresponding simulated values. meanWQ_o and meanWQ_e stand for the average observed and estimated groundwater quality parameters, respectively.

RESULTS AND DISCUSSION

For ANN implementation, first the number of hidden neurons was considered as twice the input numbers, according to Bhattacharyya & Pendharkar (1998). Then, various particle swarm/population sizes were tried. According to Geethanjali *et al.* (2008), the typical ranges for the number of particles are 20–40, and 10 particles are large enough to get good results for most of the problems.

In the present research, four different particle sizes, i.e., 10, 20, 30, and 40 were tried with 10,000 iterations for the ANN-PSO models, with hidden node number of 18 (2×9 inputs). Then, the hidden node number was decreased to the number of inputs (nine nodes). The sensitivity analysis of different ANN-PSO models with respect to hidden node numbers is presented in Table 3. From the table it is seen that the RMSE values vary between 3.19 mg/L and 9.43 mg/L for the SO_4 and between 3.87 and 8.03 for the SAR. It is clear that the ANN-PSO is very sensitive to hidden node numbers. The model with 16 hidden nodes

Table 3 | Sensitivity analysis of different ANN-PSO models with respect to hidden node number

	Training			Validation			Test		
Hidden node number	RMSE	MAE	R^2	RMSE	MAE	R^2	RMSE	MAE	R^2
SO_4									
18	2.90	1.88	0.846	3.95	2.54	0.766	3.76	2.46	0.854
17	2.64	1.77	0.873	5.66	4.84	0.852	7.38	5.86	0.847
16	2.59	1.76	0.877	3.20	2.32	0.847	3.19	2.46	0.888
15	3.01	2.06	0.834	10.2	9.61	0.751	9.14	8.51	0.832
14	3.00	2.02	0.835	8.52	7.92	0.798	9.43	8.59	0.797
13	2.53	1.76	0.884	4.21	3.27	0.776	3.79	3.14	0.909
12	2.49	1.71	0.887	4.03	2.78	0.766	3.43	2.64	0.897
11	2.73	1.85	0.863	3.62	2.42	0.812	3.31	2.11	0.874
10	2.71	1.74	0.865	6.05	5.44	0.833	6.06	5.26	0.877
9	2.72	1.80	0.864	5.59	5.20	0.843	4.51	3.43	0.847
SAR									
18	3.05	1.98	0.802	4.71	3.03	0.739	3.87	2.61	0.810
17	3.11	2.03	0.793	10.1	9.32	0.549	6.89	6.11	0.759
16	3.67	2.48	0.712	5.20	2.95	0.512	4.55	2.95	0.709
15	3.33	2.21	0.763	6.64	5.64	0.733	5.11	4.46	0.801
14	3.29	2.11	0.768	4.90	3.73	0.711	4.01	3.06	0.784
13	3.06	2.02	0.801	4.81	3.25	0.719	4.12	3.31	0.830
12	3.17	2.09	0.787	4.91	3.08	0.701	5.06	3.87	0.807
11	3.34	2.23	0.760	9.73	8.89	0.636	8.03	7.20	0.721
10	3.12	2.01	0.796	6.13	5.18	0.695	5.24	4.45	0.781
9	2.76	1.72	0.839	6.58	5.64	0.725	5.18	4.42	0.804

presents the best results in estimating SO_4 (the lowest RMSE and the highest R^2 values). In the case of SAR, however, the ANN-PSO model with 18 hidden nodes outperforms the other models.

Similarly to the ANN-PSO models, four different population sizes of 10, 20, 30, and 40 with 10,000 iterations were tried for the ANN-DE models and hidden node number was set to 18. Then, the hidden node number was decreased to the number of inputs (nine nodes). The sensitivity analysis of different ANN-PSO models with respect to hidden node numbers is presented in Table 4. From the table it is clear that the ANN-DE is not very sensitive to hidden node numbers. Similarly to the ANN-PSO, the ANN-DE model comprising 16 hidden nodes presents the best performance in modeling SO_4. In estimating SAR, however, the ANN-DE model with 12 hidden nodes performs better than the other models.

Training, validation, and test results of the ANN-PSO models are given in Table 5. It is clear from the table that the models' accuracy decreases by increasing swarm size of training data, while for the validation and test stages, the accuracies are fluctuating. Analyzing the error statistics presented in Table 3 shows that the ANN-PSO with 30 swarm size has the lowest RMSE (3.76 mg/L) and MAE (2.46 mg/L) values in estimating SO_4 in the test stage; ANN-PSO with 40 swarm size produced the most accurate results for estimating SAR.

Table 6 sums up the training, validation, and test results of the ANN-DE models. It is apparent from the table that the ANN-DE presents the lowest RMSE (2.91 mg/L) and MAE (1.88 mg/L) in estimating SO_4 in the test period for the 30 population size (PS), while ANN-DE with 40 PS provided the best accuracy in estimating SAR, similar to the ANN-PSO.

Table 4 | Sensitivity analysis of ANN-DE models with respect to hidden node number

	Training			Validation			Test		
Hidden node number	RMSE	MAE	R^2	RMSE	MAE	R^2	RMSE	MAE	R^2
SO_4									
18	2.76	1.86	0.868	2.92	1.95	0.854	2.91	1.88	0.880
17	2.28	1.54	0.910	3.65	1.90	0.799	2.85	1.78	0.885
16	2.11	1.43	0.923	2.88	1.72	0.872	2.22	1.64	0.932
15	2.16	1.39	0.933	3.33	1.52	0.836	2.89	1.60	0.902
14	2.18	1.53	0.930	4.01	2.23	0.809	2.93	1.95	0.898
13	2.28	1.45	0.905	3.53	1.93	0.790	2.90	1.78	0.878
12	1.91	1.12	0.934	3.25	1.42	0.826	2.62	1.41	0.901
11	1.99	1.28	0.929	2.60	1.54	0.884	2.34	1.57	0.923
10	2.51	1.89	0.892	3.22	1.95	0.818	2.85	1.99	0.885
9	2.09	1.42	0.922	3.10	1.64	0.833	2.59	1.54	0.903
SAR									
18	1.98	1.48	0.920	2.55	1.62	0.865	2.22	1.60	0.896
17	1.90	1.41	0.930	2.83	1.71	0.834	2.42	1.59	0.874
16	2.11	1.43	0.905	3.80	1.83	0.703	2.46	1.63	0.862
15	2.15	1.55	0.918	2.82	1.47	0.831	2.27	1.42	0.883
14	2.02	1.36	0.921	3.48	1.68	0.763	2.91	1.70	0.829
13	2.01	1.29	0.914	3.78	1.72	0.714	2.67	1.68	0.849
12	1.84	1.29	0.935	3.18	1.62	0.786	2.11	1.35	0.902
11	2.00	1.38	0.925	3.67	1.85	0.725	2.82	1.75	0.839
10	1.88	1.40	0.927	2.05	1.46	0.911	2.24	1.57	0.886
9	1.75	1.23	0.937	2.20	1.48	0.898	2.32	1.70	0.886

Comparison of Tables 5 and 6 clearly shows that the ANN-DE performs better than the ANN-PSO in estimating SO_4 and SAR in all cases. The obtained results revealed that selecting the number of neurons as twice that of the input numbers may not give the optimal results, and should be obtained through a trial and error process.

The optimal ANN-PSO and ANN-DE models are compared in Table 7. From the table it is seen that the ANN-DE models give more accurate results than the ANN-PSO models for all training, validation, and test stages.

Figure 3 compares the time series of the observed and estimated SO_4 values obtained by ANN-DE and ANN-PSO models during the test period. It is clear from the figure that the values produced by the ANN-DE model are closer to the observed values than those of the ANN-PSO model. Scatterplots of the observed vs. simulated SO_4 values during the test period are also compared in Figure 4. Assuming the fit line equation as $y = ax + b$, the a and b coefficients of the ANN-DE model are closer to 1 and 0, respectively, with a higher R^2 value (0.931), which demonstrates the superiority of the ANN-DE model. Time variation and scatter plots' comparison of the ANN-DE and ANN-PSO in SAR modeling are shown in Figures 5 and 6. Similarly to the SO_4 modeling, ANN-DE is superior to the ANN-PSO in simulating SAR.

Further, the results were tested by using one-way analysis of variance (ANOVA) for verifying the robustness of the optimum ANN-DE and ANN-PSO models. Both tests were set at a 95% significance level. Thus, differences between the observed and simulated SO_4 and SAR values were considered as significant differences when the resultant significance level (p) was lower than the 0.05 by use of

Table 5 | Comparison of different ANN-PSO models with different swarm sizes

	Training			Validation			Test		
Swarm size	RMSE	MAE	R^2	RMSE	MAE	R^2	RMSE	MAE	R^2
SO_4									
10	3.87	2.72	0.750	6.84	6.16	0.746	5.66	4.86	0.690
20	3.21	2.19	0.813	6.93	6.23	0.794	7.75	6.75	0.801
30	2.90	1.88	0.846	3.95	2.54	0.766	3.76	2.46	0.854
40	2.61	1.73	0.875	6.11	5.66	0.858	7.83	7.22	0.864
SAR									
10	5.26	3.74	0.442	5.83	4.07	0.428	5.44	4.18	0.498
20	4.50	3.14	0.565	10.5	9.46	0.522	9.36	8.33	0.586
30	4.38	3.02	0.588	5.42	3.29	0.403	5.50	3.92	0.590
40	3.05	1.98	0.802	4.71	3.03	0.739	3.87	2.61	0.810

Table 6 | Comparison of different ANN-DE models with different swarm sizes

	Training			Validation			Test		
Population Size	RMSE	MAE	R^2	RMSE	MAE	R^2	RMSE	MAE	R^2
SO_4									
10	2.53	1.79	0.884	5.80	2.29	0.564	3.17	2.15	0.854
20	2.31	1.63	0.902	3.68	1.99	0.782	3.01	1.99	0.868
30	2.76	1.86	0.868	2.92	1.95	0.854	2.91	1.88	0.880
40	2.50	1.73	0.886	2.88	2.01	0.852	3.03	2.20	0.869
SAR									
10	2.05	1.39	0.912	3.27	1.73	0.780	2.44	1.54	0.867
20	2.05	1.42	0.919	3.25	1.78	0.793	3.00	1.67	0.814
30	1.83	1.37	0.931	2.87	1.52	0.829	2.69	1.62	0.837
40	1.98	1.48	0.920	2.55	1.62	0.865	2.22	1.60	0.896

Table 7 | Comparison of the optimal ANN-PSO and ANN-DE models

		Training			Validation			Test					
Model	Hidden node number	*RMSE*	*MAE*	R^2	*RMSE*	*MAE*	R^2	*RMSE*	*MAE*	R^2	Computational cost (iterations)	Run time (s)	Convergence speed (iteration/s)
	SO_4												
ANN-PSO	16	2.59	1.76	0.877	3.20	2.32	0.847	3.19	2.46	0.888	1,000	23	43
ANN-DE	16	2.11	1.43	0.923	2.88	1.72	0.872	2.22	1.64	0.932	950	21	45
	SAR												
ANN-PSO	18	3.05	1.98	0.802	4.71	3.03	0.739	3.87	2.61	0.810	1,200	28	43
ANN-DE	12	1.84	1.29	0.935	3.18	1.62	0.786	2.11	1.35	0.902	1,100	26	42

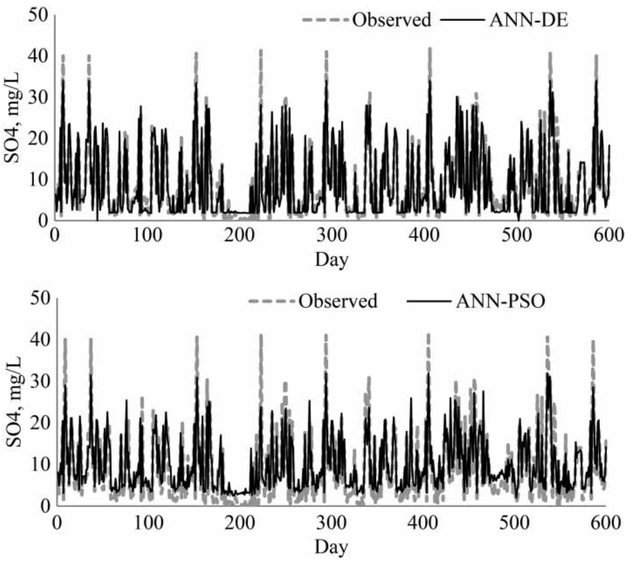

Figure 3 | Observed vs. estimated SO_4 values of ANN-DE and ANN-PSO models in the test stage.

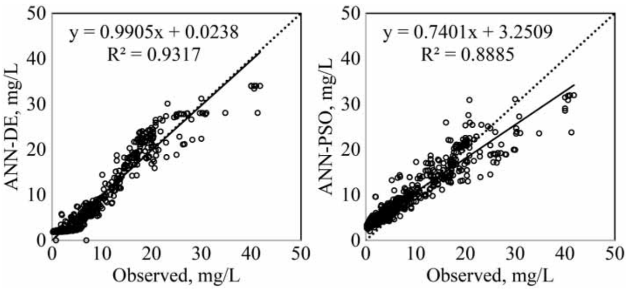

Figure 4 | Scatter plots of the observed vs. simulated SO_4 values by ANN-DE and ANN-PSO models in the test stage.

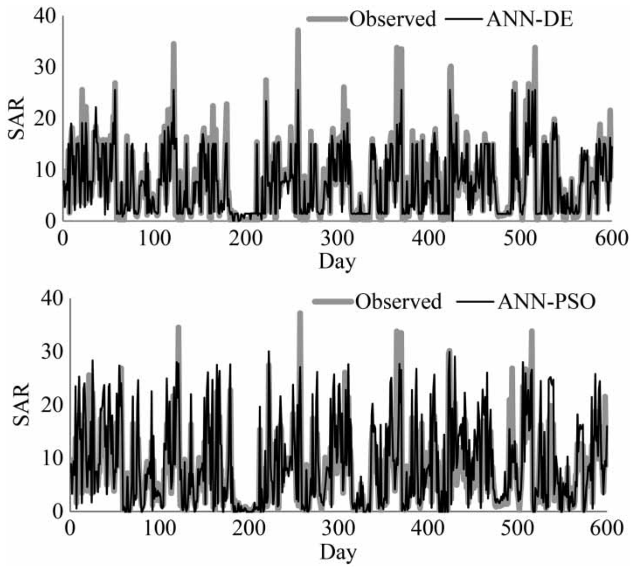

Figure 5 | The observed and estimated SAR values by ANN-DE and ANN-PSO models in the test phase.

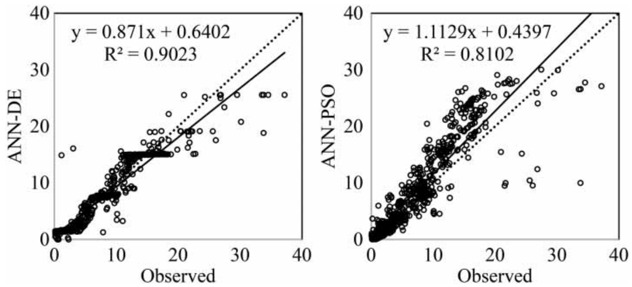

Figure 6 | The scatter plots of the observed and estimated SAR values by ANN-DE and ANN-PSO models in the test phase.

two-tailed significance levels. The test statistics are given in Table 8. The ANN-DE model yields a small testing value with a high significance level for the ANOVA in the case of both the SO_4 and SAR modeling. According to the test results, the ANN-DE seems to be more powerful than the ANN-PSO in this case.

Table 8 | ANOVA results for the optimum ANN-DE and ANN-PSO models

	SO_4		SAR	
	F-statistic	Resultant significance level	*F-statistic*	Resultant significance level
ANN-DE	0.0159	0.8991	0.8980	0.3431
ANN-PSO	4.579	0.0325	9.1861	0.0024

CONCLUSIONS

This paper presents particle swarm optimization (PSO) and differential evolution (DE)-based ANN approaches for estimation of groundwater quality parameters (SO_4 and SAR). Two powerful bio-inspired algorithms, PSO and DE, were compared in order to determine which one is more suitable to train an ANN. This is very important because the training of an ANN is one of the key issues to obtain a good generalization. Application of PSO- and DE-based ANN to estimate groundwater quality is a novel research area. A comparison between an ANN trained with the PSO and DE algorithms was performed when applied to estimate groundwater quality. The outcomes and finding of this study indicated that both ANN-PSO and ANN-DE are suitable approaches for simulating groundwater quality. However, it can be observed that the DE-based model exhibits better performance in the training as well as validation and test stages than those of the PSO-based model. The present study used ANN-PSO and ANN-DE models for estimating SAR and SO_4 using other qualitative parameters. Further studies should be carried out using limited inputs to verify the generalization of the developed models. Nonetheless, studies around relating SO_4 pollution with certain industrial discharges or with rainfall intensity would be of interest.

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