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Comparison of Optimal Artificial Neural Network Models for Groundwater Nitrate Simulation (Case Study: Behbahan Plain)

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Abstract

Groundwater is the most important water resource for drinking and agricultural usage especially in arid and semi-arid regions. So, it is important to note its quality. Nitrate is one of the groundwater pollutants which is mostly derived from agricultural and wastewater sources. Since nitrate determination using sampling was very expensive and limited, it is necessary to use new prediction methods like artificial neural network. The use of artificial neural networks in hydrological studies of the last decade shows that these models have a high ability to discover the relationship between data and recognize patterns. The success of neural network models in estimating different parameters of water sources has always been emphasized by different researchers.

1. Introduction

Groundwater is very important in arid and semi-arid areas such as Iran, where the average rainfall is less than a third of the average rainfall in other parts of the world, and plays a significant role as a reservoir for fresh water. These resources become more important in hot and dry areas where rainfall is less. Contamination of underground water resources is a serious threat in these areas and land use should be defined according to the potential and risk of contamination of aquifers. In some cases, natural processes seriously cause pollution, but most of the human concerns about groundwater pollution are caused by human activities. Nitrogen exists in various forms in nature and is transformed from one form to another by various processes. Commercial urea fertilizers are converted to NH4+ in water. In aerobic conditions, NH4+ is oxidized and turns into nitrate (NO3-). Nitrate is the most stable form of nitrogen after gaseous N2 in most groundwaters [1]. A simple cycle of nitrogen is shown in figure 1. Nitrogen enters the soil from three sources: atmospheric, organic and inorganic fertilizers. In the soil area, nitrogen is converted into nitrate and ammonium and a part of it is consumed by plants, a part is converted into nitrite by bacteria and finally into nitrogen gas and returns to the atmosphere and another part is absorbed by clay minerals. The remaining nitrate passes through the unsaturated zone and enters the underground water tables. Nitrate in groundwater is either decomposed by bacteria and returns to the atmosphere through the unsaturated zone and soil layer, or it enters surface water, or it reaches various uses, including drinking, through exploitation wells [2]. Nitrate is soluble in water, it is not absorbed by soils rich in clay and it originates as a widespread and common pollutant in groundwater from human and urban activities [3,4]. The amount of nitrate concentration in underground water usually varies between 0.1 and 10 mg/liter, but its amount ranges from about 0.1 to 0.3 in rainwater to more than 600 mg/liter in groundwater affected by nitrate fertilizers [5]. Accurate and timely prediction of the quality parameters of available water resources can be

considered as a key point in planning, management and optimal utilization of water resources. Measuring these parameters in high volume is time-consuming, expensive and requires high accuracy, therefore, some indirect methods to estimate these parameters are becoming more visible. In the field of water quality management, many models have been developed, and these models require many input parameters such as hydrological, meteorological data, etc., which are either difficult to access or their measurement requires spending a lot of money and time [6]. Therefore, obtaining reliable methods of predicting the qualitative parameters of underground water in order to plan the timely and correct use of water resources is of particular importance. The use of artificial neural networks in hydrological studies of the last decade shows that these models have a high ability to discover the relationship between data and recognize patterns. The success of neural network models in estimating different parameters of water resources has always been emphasized by different researchers [7,8]. The researchers considered nitrate as a function of the ions present in groundwater and were able to predict nitrate with high accuracy by modeling with artificial neural network method and considering 6 input characteristics [9]. In [10], the nitrate concentration has been investigated in the underground water wells of Haran Plain in Turkey and predicted the nitrate concentration of the underground water with high accuracy using the ANN technique with the Lunberg Marquardt algorithm. the high ability of neural networks in estimating water quality indicators of Johor River in Malaysia in estimating EC, TDS and turbidity is emphasized in [6]. Using two artificial neural network models and a hybrid neural network model to estimate total dissolved solids, electrical conductivity and sodium absorption ratio of Jajroud and Qarasu rivers in Kermanshah and showed the high capability of the hybrid model compared to the neural network model [11]. Also, [12] simulated the qualitative parameters of underground water in Kashan plain using artificial neural network model. The result of the research showed the high accuracy of the neural network model in the simulation. In another study, the researchers used gene expression and fuzzy-neural programming methods to investigate the short-term fluctuations of the underground water level of two wells in Turkey [13]. The results obtained from his research indicated the appropriateness of two methods in investigating water level fluctuations. In a similar research, the gene expression programming model has been used for estimating evaporation and transpiration in a region in Africa and reported the accuracy of this model as acceptable [14]. using the neural network model and optimizing the results of this model based on genetic algorithm optimization, have predicted nitrate values in Birjand Plain [15,16]. The results of this research showed the reliability of this model in predicting nitrate with a correlation coefficient of 0.83. Sayadi Shahraki also confirmed the ability of the genetic algorithm in hydraulic head simulation of sugarcane cultivation and industry in Dabal Khazai [17]. By reviewing the past studies, it seems that simulation-optimization studies of qualitative parameters have a special place. Therefore, the aim of the current research is to simulate the groundwater nitrate of Behbahan Plain, using the particle swarm optimization algorithm and the genetic algorithm in the MATLAB software environment and comparing their results with the values measured in the field.

2. Materials and Methods

2.1. Study area: Behbahan plain aquifer with an area of about 430 square kilometers and geographic coordinates ″15'40°30 to ″45'35°N latitude and ″56'4°50 to ″49'23°E longitude, is located in the southeastern part of Khuzestan province. The climate of the study area has been determined as semi-arid by the Dumarten method. The average annual rainfall in the plain area is 450.2 mm, the absolute minimum temperature is -1.5 °C and the absolute maximum temperature is 50.5 °C. The maximum height above sea level is 560 meters and the minimum is 257 meters. Figure (2) shows the location of the studied area.

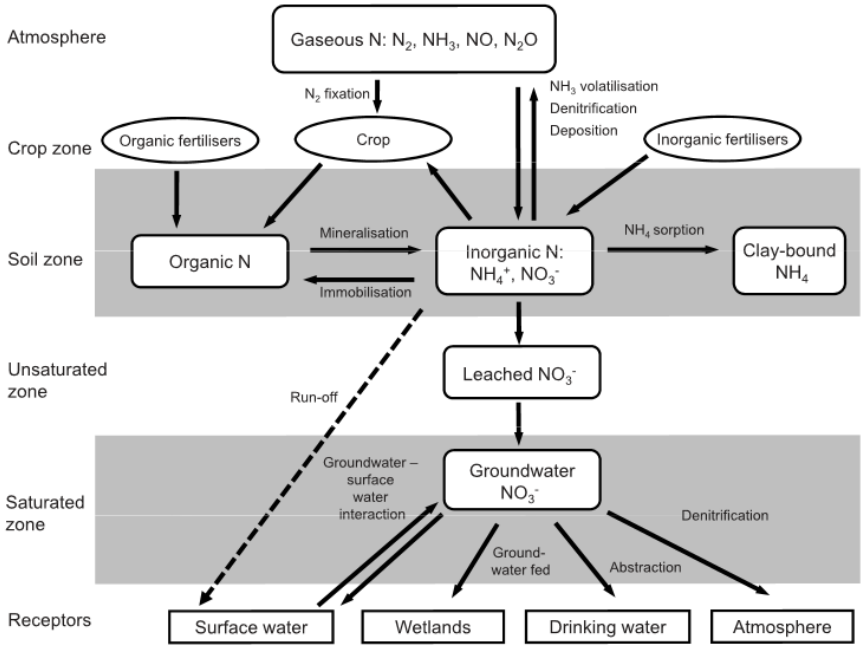

Figure 1. Simplified nitrogen cycle (Stuart et al., 2011)

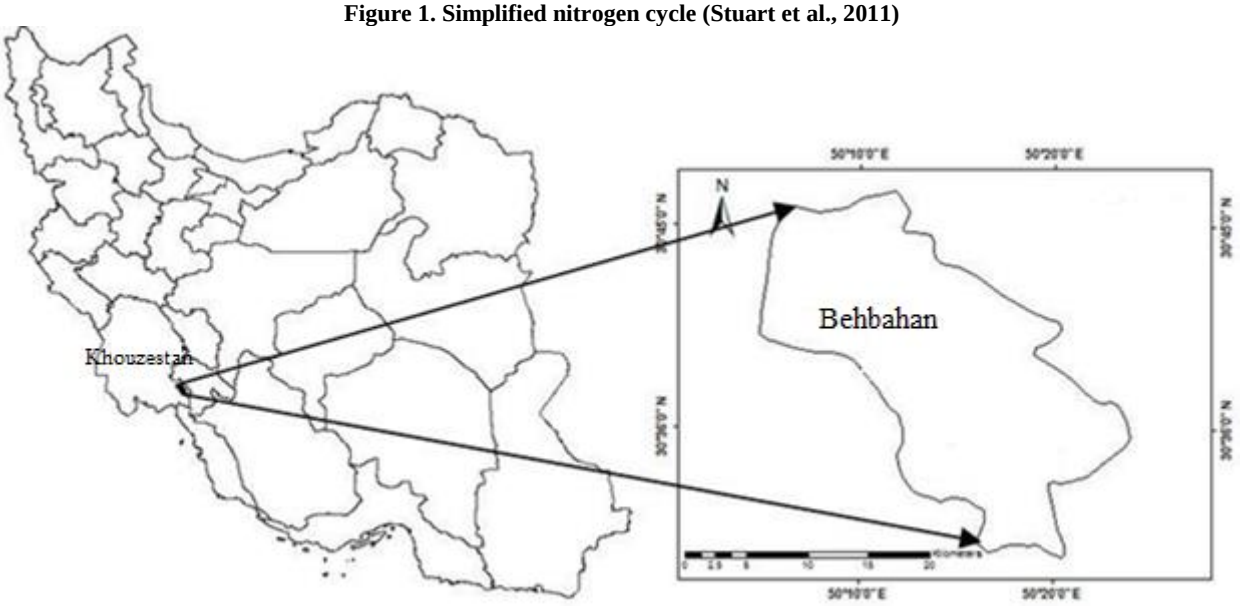

Figure 2. Geographical location of the study area

2.2. Particle Swarm Optimization Algorithm (PSO): The principle of this algorithm is based on the fact that swarm members in a search space are adopted towards the past successful regions and also are affected from the success of the neighboring members. This idea is explicitly stated as follows:

Each swarm member is called a "particle" which shows a potential solution, and in search space, changes the location and updates its velocity based on the flight experiences of itself and its neighboring particles, which help it to gain a better position. Particle i is shown as $X_i = (x_{i1}, x_{i2}, \dots, x_{iD})$. The situation with the best fitting function will be recorded as the best current position. This position is considered as $P_i = (p_{i1}, p_{i2}, \dots, p_{iD})$ and the corresponding fitting function is called and recorded as $Pbest_i$. The best general position in the swarm is related to the best fitting function, and called $Gbest_i$ and recorded as $P_g = (p_{g1}, p_{g2}, \dots, p_{gD})$. Velocity or the rate of position change of particle i, is shown as $V_i = (v_{i1}, v_{i2}, \dots, v_{iD})$. During the replication process, velocity and position of the particle i will be updated in accordance with the following equation:

$$V_{id}(t+1) = K\left(V_{id}(t) + rand(0,\varphi_1).\left(P_{id}(t) - X_{id}(t)\right) + rand(0,\varphi_2).\left(P_{gd}(t) - X_{id}(t)\right)\right) \quad (1)$$

$$X_{id}(t+1) = X_{id}(t) + V_{id}(t+1) \qquad d = 1,2,\dots,D \quad (2)$$

$$K = \frac{2}{\varphi - 2 + \sqrt{\varphi^2 - 4\varphi}} \quad (3)$$

in where $\varphi = \varphi_1 + \varphi_2$

K is the contraction factor and a function of φ_1 and φ_2 and constant acceleration values of φ_1 and φ_2 shows the weighting of particles random acceleration for tendency towards the personal and global best position. $\mathrm{rand}(0,\varphi_1)$ and $\mathrm{rand}(0,\varphi_2)$ functions, respectively produce random numbers in the range of $[0,\varphi_1]$ and $[0,\varphi_2]$. According to equation (2), particles current flight velocity includes three parts: The first part indicates the previous velocity of the particle, and the second and the third parts show single particle and swarm model. In single particle model, each member is separated and used personal thoughts and experiences independently; while in the swarm model, members move towards success based on the effective experiences of their neighbors [18]. Although the PSO algorithm is able to quickly find the area of feasible solution, but the convergence rate will be severely reduced getting to this area. To solve this problem, equation (1) is amended as follows:

$$V_{id}(t+1) = \omega\left(V_{id}(t) + c_1 rand(0,\varphi_1).\left(P_{id}(t) - X_{id}(t)\right) + c_2 rand(0,\varphi_2).\left(P_{gd}(t) - X_{id}(t)\right)\right) \quad (4)$$

In the above equation, ω, c_1 and c_2 respectively represent inertia weight, a positive parameter called cognitive parameter, and a positive parameter called social parameter.

Using inertia weight parameter leads to a compromise between global and local discovery capabilities of the category. A great inertia weight is a stimulus to enlarge the amount of velocity vector of particles throughout the solution spaces (moving towards solution spaces of the search space not experienced previously), while a smaller inertia weight narrows the solution spaces in the current small area. In fact, lower weight makes the search continue with higher accuracy in areas experienced in the past. A proper selection of ω ensures the establishment of the optimum balance between local and global solution spaces and consequently increases the efficiency of the algorithm. Thereby the amount of ω is determined equal to one at the beginning of the search, and gradually goes to zero.

2.3. Genetic algorithm (GA): A genetic algorithm is an algorithm that imitates the process of natural selection. They help solve optimization and search problems. GA are part of the bigger class of evolutionary algorithms. GA imitate natural biological processes, such as inheritance, mutation, selection and crossover.

GA is a search technique often used in computer science to find complex, non-obvious solutions to algorithmic optimization and search problems. GA is global search heuristics and is good at solving problems that include timetabling and scheduling. They have also been applied to engineering. GA is inspired by genetic science and Darwin's theory of evolution and is based on survival of the fittest or natural selection. A common application of genetic algorithm is to use it as an optimizing function. In the GA, each person from the population is introduced as a chromosome. Chromosomes become more complete during several generations. In each generation, chromosomes are evaluated and according to their value, they find the possibility of survival and reproduction. generation in the discussion of genetic algorithm is carried out with hybrid and mutation operators. Top parents are selected based on a fitness function. At each stage of genetic algorithm execution, a group of search space points are subject to random processing. In this way, a sequence of characters is attributed to each point and genetic operators are applied on these sequences. Then the obtained sequences are transformed to obtain new points in the search space. Finally, based on the value of the objective function at each of the points, the probability of their participation in the next stage is determined [19]. Before a GA can be implemented, a suitable encoding (or representation) for the given problem must first be found. Also, a fitness function should be devised to assign a value to each coded solution. During execution, parents are selected for reproduction and combined using the fusion and mutation operators to produce new offspring. This process is repeated several times until the next generation of the population is produced. Then this population is examined and if the convergence criteria are met, the above process is terminated. In this research, the initial population number was 100, the maximum generation was 150, and the number of repetitions was 200 rounds.

2.4. Artificial Neural Network Model (ANN): The key element of this pattern is the new structure of the data processing system consisting of a large number of the data processing systems consisting

of many elements (neurons) with strong internal communications that work harmoniously together to solve specific problems. Processing the experimental data, artificial neural networks transfer the knowledge or the law behind the data to the network structure; a training process. Using computer programming knowledge, data structures can be designed which act as a neuron. Then it can be trained by creating a network of interconnected artificial neurons, creating a training algorithm for network and applying the algorithm to the network. In general, a neural network is made up of three layers:

The input layer only receives data and acts the same as independent variable. Thus the number of input layer neurons is determined based on the nature of the problem and depends on the number of independent variables. The output layer acts similar to a dependent variable and the number of its neurons depends on the number of dependent variables. But the hidden layer, unlike the input and output layers, represents nothing and is only an intermediate result in the process of calculating the output value [20-21].

2.4.1. Objective function and used decision variables: The concept of neural network training is actually determining the values of weights and biases in the network. As mentioned earlier, in the usual neural network, the error back propagation method is used to train the network, the main disadvantage of which is premature convergence to the local optimum. In optimization using PSO, optimization variables in training a neural network include weights and biases related to the network. The work process is as follows: first, N location vectors X_i , where N is equal to the number of team members, are randomly generated. The group population is usually 4 to 5 times the number of optimization variables. The neural network is formed by the weights and biases obtained from the variables of these vectors and the error obtained from each execution is considered as the fitness rate of the variable vector of that network. This process is repeated until the final convergence is achieved. The aim of the final convergence is to reach the optimal location vector (values of optimal weights and biases), in such a way that the training error is minimized. Therefore, the objective function that should be minimized in this optimization is the amount of prediction error. If the number of layers is 3 and the number of neurons in the hidden layer is 7, so the number of weights is the number of weights between the input and the hidden layer + the number of weights between the hidden layer and the output (the number of inputs * the number of neurons in the hidden layer + the number of neurons hidden layer = 10*7+7=77) and the number of biases is the total number of neurons, which are 8. Therefore, the total number of decision variables is 85 and each group of population includes 5 vectors with this dimension.

The purpose of standardizing the input data of the neural network model is to normalize them. The best situation for neural networks is when all inputs and outputs are between zero and one. To normalize the data, the mapminmax function was used in MATLAB software. The next step includes determining the model, specifying the architecture, the optimal number of iterations, determining the number of hidden and input layer neurons, the number of layers, and determining the appropriate stimulus function for the desired neural network model (in this research, the optimal number of iterations is 27,000, the number of layers is 3 and sigmoid tangent driving function is used). The next step is to train the network, which means determining the amount of weights and biases with a part of the data by optimization algorithms of particle swarm and genetics. Then the evaluation and testing of the network with the rest of the data is done by statistical parameters to evaluate the used algorithms and finally the output and simulation results are displayed by the model.

In this research, 85% of the data were considered for training and 15% of the data were considered for validating the model.

2.5. Model evaluation criteria: To determine the accuracy of the models the values of Root Mean Square Error ($RMSE$), Mean Absolute Error (MAE) and Determination Coefficient (R^2) was used:

$$RMSE = \sqrt{\frac{1}{n}\sum(y_{observed} - y_{predicted})^2} \quad (5)$$

$$MAE = 100 * \frac{1}{n}\sum|y_{observed} - y_{predicted}| \quad (6)$$

$$R^2 = 1 - \frac{\sum(y_{predicted} - y_{observed})}{\sum y_{predicted}^2 - \frac{y_{observed}}{n}} \quad (7)$$

In the above equation, $y_{predicted}$, $y_{observed}$ and n are respectively the representatives of predicted values, observed values and the number of data. As the accuracy of the prediction model increases, RMSE and MAE tend to zero and R^2 approaches one.

3. Results and discussion

In this study, quality data of Behbahan plain during the years 2014 to 2018 was used in order to simulate groundwater nitrate. Input information to the models for simulating nitrate (NO_3^-) on a monthly basis and including electrical conductivity (EC), calcium (Ca^{2+}), magnesium (Mg^{2+}), sulfate

(SO_4^{2-}), bicarbonate (HCO_3^-), chlorine (CL^-), potassium (K^+), hardness (TH) and pH (pH). Input characteristics of quality parameters are shown in table (1).

Table 1 – Statistical Profile groundwater quality parameters Behbahan Plain

Water quality parameters	unit	minimum	maximum	average	Standard deviation
NO_3^-	mg/lit	1.28	112.4	24.95	17.41
EC	µs/cm	431	7457	2697.47	1594.08
Ca^{2+}	mg/lit	1.21	42.01	13.83	9.88
Mg^{2+}	mg/lit	0.5	28.51	6.69	5.2
SO_4^{2-}	mg/lit	0.79	47.86	26.88	12.96
HCO_3^-	mg/lit	1.04	5.88	3.47	0.9
CL^-	mg/lit	0.4	34.55	18.26	6.03
K^+	mg/lit	0.01	2.01	0.133	0.174
TH	mg/lit	51.5	285.03	938.3	409.7
pH	…	6.05	8.1	7.23	0.35

According to table 1, the highest and lowest values of nitrate concentration in groundwater are 112.4 and 1.28, respectively. While the maximum permissible and desirable nitrate in drinking water according to the national standard of Iran (No. 1053) is equal to 50 mg/lit [22]. The most important factor of nitrate entering this plain is the agricultural activities above the aquifer and the significant use of ammonia and potash nitrate fertilizers. In the flood irrigation method, about 20% of the total amount of irrigated water is returned to the groundwater, which is used in many areas of Behbahan plain. Also, the nitrogen compounds of urban and rural wastewaters are another factors of the high nitrate concentration in this plain. The high concentration of nitrate is due to the nitrification process [23]. Nitrogenous compounds enter the aquifer through urban and rural sewage and are converted into nitrates during the nitrification process. The high permeability of the sandy aquifer provides favorable conditions for the vertical transfer of oxygen to the deep parts of the aquifer [24]. Due to the presence of sufficient oxygen, the nitrification reaction is possible, and most of the studied area is alluvial, and in alluvial aquifers with abundant oxygen, nitrification takes place and ammonia is converted into nitrate [16]. The mentioned reasons are consistent with the researches who conducted studies on nitrate concentration in drinking water of Tehran and Ardabil [25,26]. Due to the importance of knowing the state of nitrate concentration in the future, the artificial neural network model with two training algorithms for particle swarm optimization and genetics has been used to simulate nitrate concentration. All the calculations of this research were done in MATLAB, Excel and SPSS.

Analyzing the degree of correlation between the input variables and the work target variable is very valuable, because it provides useful information about the dependence of each of the input parameters on the target parameter. Table 2 shows the correlation between nitrate and other input parameters of the model.

Table 2 – The correlation matrix between nitrate and model input variables

Parameter	pH	TH	K^+	CL^-	HCO_3^-	SO_4^{2-}	Mg^{2+}	Ca^{2+}	EC
NO_3^-	-0.39	0.23	0.889^{**}	0.157	0.51^{**}	0.41	0.15	0.68^{**}	0.72^{**}

According to table 2, among all the input parameters of the model, the highest correlation with nitrate at the confidence level of 0.89 is related to K^+ due to the use of potash fertilizers, which is based on the results of the research in [27] Nitrate of Zidon plain corresponds. In addition to K^+, EC and Ca^{2+} have shown a high correlation at the confidence level of 0.99 compared to nitrate.

Different networks were formed with different number of neurons and repetitions. To avoid excessive learning and reduce errors, the optimal number of repetitions in the neural network model should be determined using evolutionary algorithms. To do this, the number of repetitions was changed from 5000 to 30000 and at the end of each step, its error was recorded. In the designed network, the error until 27,000 iterations showed a downward trend and then an upward trend. Therefore, the optimal number of repetitions was chosen as 27,000. In the designed neural network model, the iteration that achieved the highest explanation coefficient in the training phase and the error below 5% was selected as the optimal iteration. Then, the number of different neurons for the hidden and input layers was considered to select the best model with the least error. The number of neurons in the hidden layer was changed from one to ten and the number of neurons in the input layer was changed from one to five, and in each step, the value of the RMSE and R^2 coefficients between the points simulated by the two algorithms and measured were calculated. The results of the repetitions of the neurons in the hidden layer are presented in table (3).

Table 3 – Results Repeat with different numbers of neurons in the hidden layer

	PSO		GA	
Number of neurons in hidden layer	**RMSE**	**R^2**	**RMSE**	**R^2**
1	0.816	0.941	0.767	0.847
2	0.828	0.942	0.789	0.861
3*	0.884	0.94	0.787	0.86
4	0.825	0.948	0.791	0.857
5	0.865	0.945	0.792	0.846
6	0.83	0.95	0.795	0.85
7*	0.811	0.957	0.794	0.869
8	0.815	0.956	0.794	0.874
9	0.822	0.938	0.798	0.879
10	0.848	0.939	0.802	0.883

According to table 3, the optimal number of neurons in the hidden layer for the optimization algorithms of PSO and GA are equal to 7 and 3, respectively. All the above steps were carried out to select the number of neurons of the input layer with the specified number of hidden layers, and the lowest error in the o PSO and GA was estimated with the number of input neurons 4.

RMSE, MAE and R^2 values were calculated between the points simulated by two algorithms (with optimal structure) and measured. Tables 4 and 5 show the statistics calculated in the training and calibration phase of the model, respectively.

Table 4 – Statistics calculated during the training phase

	PSO			**GA**		
Parameter	**RMSE**	**MAE**	**R^2**	**RMSE**	**MAE**	**R^2**
NO_3^-	0.06	0.2	0.997	0.11	0.97	0.992

Table 5 – Statistics are calculated between the measured and simulated for calibration

	PSO			**GA**		
Parameter	**RMSE**	**MAE**	**R^2**	**RMSE**	**MAE**	**R^2**
NO_3^-	0.09	0.74	0.989	0.39	1.07	0.971

According to table (4) and (5), the highest accuracy in the simulation of underground water nitrate in Behbahan Plain is related to the particle swarm optimization algorithm, so that the RMSE and MAE values are the lowest and the R^2 index is the highest compared to the genetic algorithm in both the training and it is also in the calibration phase. PSO operates on the basis of search, and in this case, it can to some extent try to randomize the selection of points with a non-deterministic method. In this method, the particles try to select and update the most optimal points in each iteration according to their positions and velocities, and for this reason, the simulation results are presented accurately. Among the other advantages of this algorithm compared to the genetic algorithm, we can mention easy implementation, low parameters of the algorithm and high convergence speed.

Figure 3 shows the fitting of the curve between the measured and simulated points of the titrate concentration using two optimization algorithms of particle swarm and genetics.

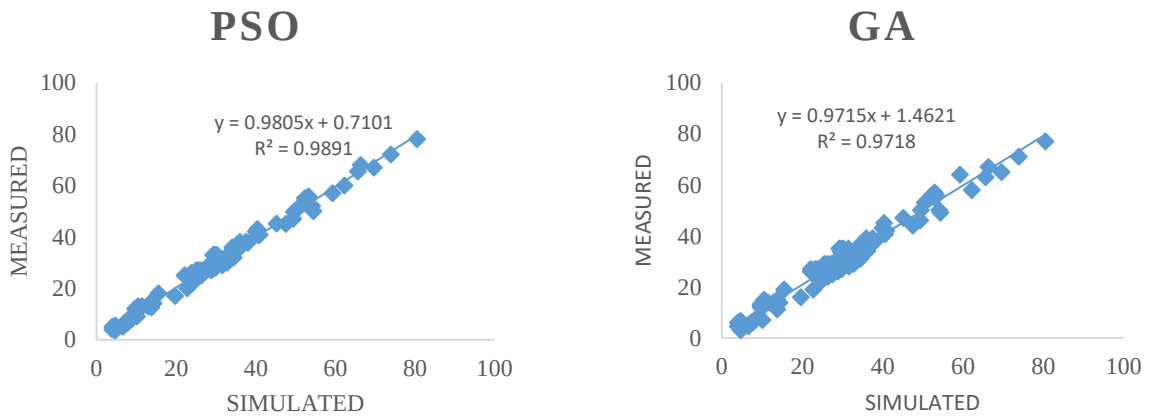

Figure 3- Scatter diagram measured and simulated nitrate concentrations using PSO and GA

In the graphs of the above figure, the R^2 value and the fitting equation between the points are specified. As mentioned, the high value of the R^2 coefficient indicates that the estimated values are close to the measured values. The linear fitting equation for each graph is defined as y=ax+b. The more the coefficient a tends towards one and the smaller the distance from one is, it indicates the better performance of the corresponding model, which according to Figure 3, the value of the coefficient a in the particle swarm optimization algorithm is higher and as a result, it performs better than the genetic algorithm in this study.

For the statistical comparison between the measured and simulated values of both algorithms, the statistical population mean comparison test was used using the t method at the error level of one percent, and the results are shown in Table 5.

Table 6 – The results of tests comparing the average

comparison	Measured and PSO+ANN			Measured and GA+ANN		
Parameter	MEAN DIFF	STD ERROR DIFF	P-value	MEAN DIFF	STD ERROR DIFF	P-value
NO_3^-	0.008	0.039	0.889 $^{n.s}$	0.029	0.042	0.707 $^{n.s}$

• n.s: there is no significant difference

Table 5 shows that the results of the GA have acceptable results for the simulation of nitrate concentration. So that there is no significant difference between the simulation values and the measured data of both algorithms at the error level of one percent.

Figures 4 and 5 show the comparison of the simulation of nitrate concentration with respect to time during the model testing period using the two used algorithms.

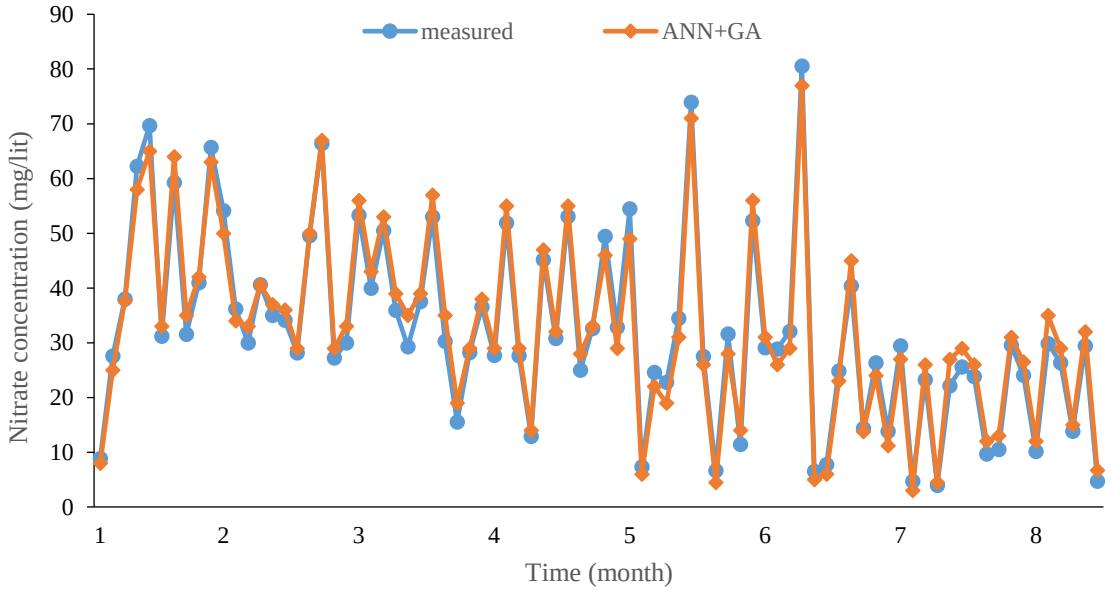

Figure 4- Compare simulate nitrate using a GA and measured data

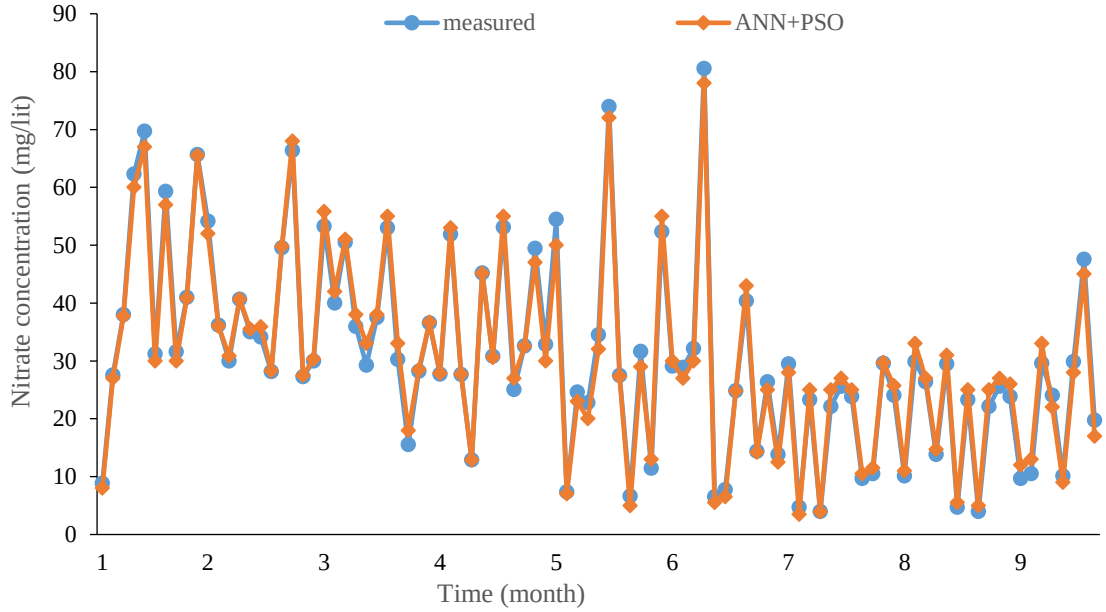

Figure 5- Compare simulate nitrate particles using PSO algorithm and measured data

4. conclusion

Artificial neural network is a suitable tool for adaptation, learning and classification of information. Many researchers have a great desire to use this tool, but they face the challenge of training neural networks. The combination of two ideas of collective intelligence and artificial neural network can be considered as an answer to this challenge. In this research, two optimization algorithms of particle swarm optimization and genetics have been used to predict nitrate concentration in Behbahan plain. The results showed that the accuracy of the particle swarm optimization algorithm is higher than the GA model. So that the values of RMSE, MAE and R^2 statistics in the training phase for the PSO algorithm were equal to 0.06 (mg/lit), 0.2 (mg/lit) and 0.997, respectively. These statistics for the GA algorithm were determined as 0.11 (mg/lit), 0.97 (mg/lit), and 0.992, respectively. In the calibration stage, the RSME parameter for PSO and GA algorithms was calculated as 0.09 and 0.39 (mg/lit), respectively. MAE statistics for these two algorithms were estimated as 0.74 and 1.07 (mg/lit), respectively, and R^2 statistics were estimated as 0.989 and 0.971, respectively. The R^2 statistic in the simulation stage for PSO and GA algorithms was 0.989 and 0.971, respectively. Also, the results of the statistical test comparing the averages between the measured and simulated data

show that there is no significant difference between any of the values predicted by the used algorithms and the measured data; So these models can be used to determine nitrate concentration in groundwater sources.

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