



Comparison of Self-Organizing Map, Artificial Neural Network, and Co-Active Neuro-Fuzzy Inference System Methods in Simulating Groundwater Quality: Geospatial Artificial Intelligence

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Abstract

Water quality experiments are difficult, costly, and time-consuming. Therefore, different modeling methods can be used as an alternative for these experiments. To achieve the research objective, geospatial artificial intelligence approaches such as the self-organizing map (SOM), artificial neural network (ANN), and co-active neuro-fuzzy inference system (CANFIS) were used to simulate groundwater quality in the Mazandaran plain in the north of Iran. Geographical information system (GIS) techniques were used as a pre-processor and post-processor. Data from 85 drinking water wells was used as secondary data and were separated into two splits of (a) 70 percent for training (60% for training and 10% for cross-validation), and (b) 30 percent for the test stage. The groundwater quality index (GWQI) and the effective water quality factors (distance from industries, groundwater depth, and transmissivity of aquifer formations) were implemented as output and input variables, respectively. Statistical indices (i.e., R squared (R-sqr) and the mean squared error (MSE)) were utilized to compare the performance of three methods. The results demonstrate the high performance of the three methods in groundwater quality simulation. However, in the test stage, CANFIS (R-sqr=0.89) had a higher performance than the SOM (R-sqr=0.8) and ANN (R-sqr=0.73) methods. The tested CANFIS model was used to estimate GWQI values on the area of the plain. Finally, the groundwater quality was mapped in a GIS environment associated with CANFIS simulation. The results can be used to manage groundwater quality as well as support and contribute to the sustainable development goal (SDG)-6, SDG-11, and SDG-13.

Keywords Ground water quality index · Training · Test · Groundwater quality map · Mazandaran plain

1 Introduction

In arid and semi-arid areas such as Iran, due to water scarcity, studies of groundwater are very important for water resources protection and planning. More than 90% of the water consumed in Iran consists of groundwater. Since Groundwater is less susceptible

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to bacterial pollution and evaporation than surface water, it is more important. In recent decades, human activities such as agriculture, manufacture, and urban development have affected groundwater quality negatively. Therefore to optimally manage water resources, it is necessary to study water quality. Water qualitative measurements and experiments are difficult, costly, and time-consuming, therefore, researchers applied various models to simulate groundwater quality (Haddad et al. 2013; Millar et al. 2019; Wu et al. 2020). Application of artificial intelligence (AI) in groundwater modeling was initiated in the early 1990s and so far, many studies have been conducted on the successful application of this method (Nikoo and Mahjouri 2013; Tongal and Booij 2018; Li et al. 2020; Maliqi et al. 2020; Pal and Chakrabarty 2020; Mosaffa et al. 2021).

Artificial neural networks (ANN) are one of the most widely used AI methods in hydrological modeling. One of the distinguishing features of the ANN method is to provide an applied solution to simulate in a water resources system (Hsu et al. 1995; Wang et al. 2010; Gholami et al. 2021; Huang et al. 2021). Later ANNs were combined with fuzzy logic methods and this resulted in the advent of neuro-fuzzy systems such as the co-active neuro-fuzzy inference system (CANFIS) (Pramanik and Panda 2010; Varvani and Khaleghi 2019). CANFIS as a multi-layer feed-forward network uses Gaussian functions for fuzzy sets and also can combine the benefits of both neural and fuzzy networks (Ullah and Choudhury 2013; Choubin et al. 2020a, b; Fang et al. 2020). Further, the self-organizing map (SOM) method or a Kohonen map is another common method in the field of AI (Kohonen 1982, 1984, 2005; Laaksonen and Honkela 2011; Mosavi et al. 2020a). It uses unsupervised, competitive learning, and then combines the goals of the projection and clustering algorithms (Klobucar and Subasic 2012). The SOM method builds a two-dimensional map (lattice) of feature space, and it is suitable to deal with noisy, non-stationary, and non-Gaussian data (Iwashita et al. 2011). A SOM is a type of ANN that is trained by using unsupervised learning to produce an output. It shows in the input space of the training samples, called a map. A SOM requires a neighborhood (i.e., the adjacent nodes) function to preserve the topological properties of the input space (Aneetha and Bose 2012). The SOM algorithm is a powerful tool to analyze the data (Aneetha and Bose 2012; Toor and Singh 2013; Singh 2014; Jassar and Dhindsa 2015).

SOM has been developed for a wide range of water resources issues and modeling for water quality assessment (Ehsani and Quiel 2008; Iwashita et al. 2011; Haider et al. 2015; Mosavi et al. 2020b). Numerous studies showed that one of the most superior classification accuracy results have been achieved by using SOM as well-justified machine learning techniques (Muller and Van Niekerk 2016; Gholami et al. 2020). The advantage of SOM compared to other methods is that in this method, the error due to the complexity of the model as well as the error related to forecasting is minimized and this model can work with less training data and less variables. However, it is sensitive to variations depending on the training data. Further, its run-time is shorter than other methods (Lin et al. 2016). Although SOM has excellent features, there are still limited studies using SOM in modeling groundwater quality in arid regions with limited daily climatic data because of its short history. Artificial intelligence-based methods can also earn better than relationships between input and output parameters (Besalatpour et al. 2014; Mosavi et al. 2020c). Each of the three methods of ANN, neural fuzzy (CANFIS) and SOM showed a high performance in hydrological modeling processes. Previous studies on water quality using ANNs (Ghose et al. 2010; Pal and Chakrabarty 2020), CANFIS (Memarian et al. 2016; Allawi et al. 2018) and SOM (Han et al. 2011; Li et al. 2020) have shown their performance in hydrological modeling.

In water quality studies, it is necessary to use an appropriate index. In recent decades, several studies have used various indices for groundwater quality investigations (Giljanovic 1999). Numerous studies have been conducted to measure the groundwater quality index (GWQI). The GWQI was introduced by Brown et al. (1970) and later improved by the Scottish Development Department (1975), following the suggestion in Horton (1965) that the various water quality data could be aggregated into one overall index (House and Ellis 1987). Gholami et al. (2015a, b) utilized statistical and GIS techniques to classify groundwater quality in Mazanmdaran plain (north of Iran). Singh et al. (2011) applied a GIS-based multi-criteria analysis by assigning weights to different water quality parameters (Pirasteh et al. 2006; Farjad et al. 2012). They grouped water quality into six classes ranging from very mild to unfit for drinking. They found that in most of the study areas, water quality varies from moderate to good except in some areas where the groundwater quality is classified as 'poor to unfit'.

In recent years, much progress in artificial intelligence techniques has been seen and applied in many cases, including environmental and water quality. The large-scale availability of high-quality and geospatial data and the advances of both hardware and software have contributed to the GIS modeling efficiency and creating smart maps. Processing the data and transforming them into computer vision and programming language incorporated with machine learning enabled the us to create applied maps (Li and Hsu 2020; Xie et al. 2020).

Three (SOM, ANN, CANFIS) have been used in several studies on modeling the quantity and quality of water. A review of previous studies showed that each of these methods has high performance in water quality modeling. We intend to evaluate their performance with similar data in order to compare their performance and determine the most efficient method, and finally to produce groundwater quality maps by automatically integrating the optimal method in a GIS. This study aims to test the use of three AI methods of and in combination with GIS to model groundwater quality. The results present the capabilities of a co-active neuro-fuzzy inference system (CANFIS), ANN, SOM, and GIS rapidly and accurately in simulate groundwater quality.

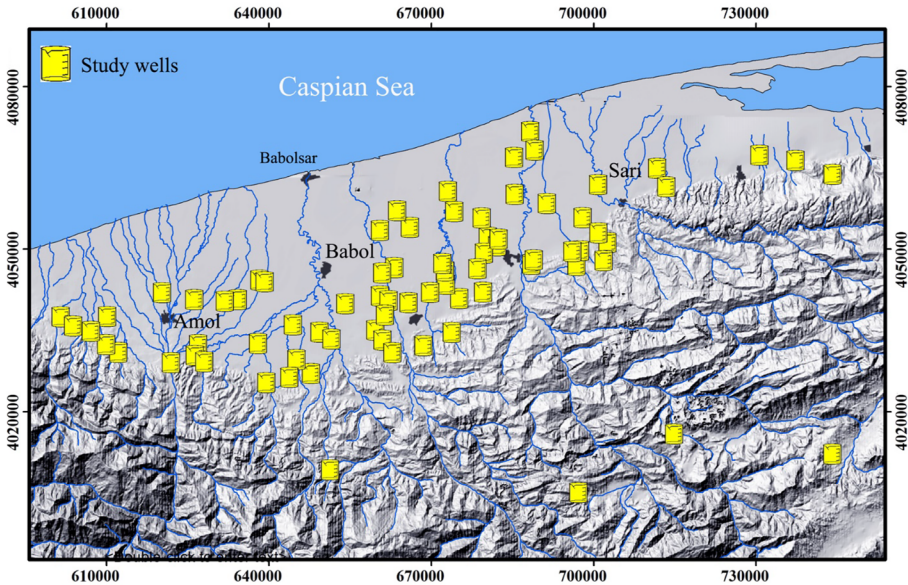
2 Materials and Method

2.1 Study Area

The study area is a plain, in the north of Iran (Mazandaran province), with an area of approximately 10,000 km² located between 35° 55' to 36° 45' N latitude and 50° 30' to 53° 50' E longitude (Fig. 1). The southern coasts of the Caspian Sea include plains made of Quaternary sediments. The study plain is located between the Caspian Sea in the north and the Alborz highlands in the south. This plain has a very low slope and its elevation varies from -27 m on the coast to 100 m in the south of the plain. Various land uses can be found, including paddy lands, residential areas, water resources, gardens and limited forest lands. Its surface water resources include rivers and wetlands, and its groundwater resources include unconfined and confined aquifers. In recent decades, due to the favorable climatic conditions and proximity to the sea, the tourism industry in this area has grown significantly. Population growth, a limited number of industries, agricultural development (use of pesticides and fertilizers) without observing environmental standards have increased pollution and reduced the quality of water



(A)



(B)

Fig. 1 Study area (A) and location of the groundwater wells (B)

resources in the study plain. Therefore, it is important to take the necessary measures for the protection of water resources.

2.2 Determination of Groundwater Quality Index

In this study, eight water quality parameters including cations and anions (K^+ , Na^+ , Ca^{2+} , Cl^- , Mg^{2+} , and SO_4^{2-}), pH, and total dissolved salt (TDS) were selected. These parameters were used for estimating the groundwater quality index. Because of the lack of microbial pollution measurements in the region, there is a limitation in defining the water quality index. Out of 200 drinking water wells in the study area, 85 wells were selected based on their existing qualitative secondary data (water quality experiments). The selected wells had adequate water quality data over a 6-year period from 2012 to 2017 compared to shorter periods for other wells. (ABFAR 2017). Estimating the groundwater quality index (GWQI) for 85 wells was done using quantitative secondary data from (i.e., 6-year data with four samples per year). The location of these drinking water wells in the study area is shown in Fig. 1. Before looking into the groundwater quality index, it is necessary to select a standard criterion to decide the parameters' greatest values. National standards of Iran for potable water quality including the eight parameters are given in Table 1.

Equation (1) was applied to estimate the groundwater quality index (GWQI) based on the standard values given in Table 1:

$$GWQI = \sum_{i=1}^8 w_i \cdot \frac{C_i}{C_{Si}} \quad (1)$$

where C_i is the concentration of the chemical parameter (mg/L), C_{Si} is the Iranian drinking water standard for each chemical parameter and w_i is the relative weight of each chemical parameter. Each parameter has a different weight in terms of its contribution to water quality. Then the corresponding weight values of the parameters were aggregated using some types of sum or mean (e.g., arithmetic, harmonic, geometric), often including individual weighing factors (Horton 1965; Melloul and Collin 1998). To estimate the final index, by aggregating all the normalized parameters, the weights of parameters in the final GWQI are defined based on their participation in the water quality determination. The weight of participation of each parameter in the final groundwater quality index depicts in Table 2.

The GWQI values were classified based on Saeedi et al. (2010) into three classes; high ($GWQI > 0.15$); low ($GWQI < 0.04$) and suitable ($0.04 < GWQI < 0.15$). GIS was applied for data collecting and processing. Different base maps were used in the GIS environment with a resolution 50 by 50 m: a digital elevation model (DEM), the transmissivity of aquifer formations, the water table depth (TAMAB 2017), residential and industrial areas using topographic maps of the region, and GWQI values using the secondary qualitative data (ABFAR 2017). Table 3 shows the factors affecting groundwater quality and the GWQI index in some drinking water wells.

Table 1 Potable water quality standards of Iran (mgr/l except pH) (Saeedi et al. 2010)

| K^+ | Na^+ | Ca^{2+} | Mg^{2+} | SO_4^{2-} | Cl^- | pH | TDS |
|-------|--------|-----------|-----------|-------------|--------|---------|------|
| 12 | 200 | 20 | 150 | 400 | 600 | 6.5–8.5 | 2000 |

Table 2 The weight of each parameter in the final GWQI (Saeedi et al. 2010)

| Parameter | Parameter's weight |
|-------------------------------|--------------------|
| K ⁺ | 0.04 |
| Na ⁺ | 0.06 |
| Ca ²⁺ | 0.15 |
| Mg ²⁺ | 0.2 |
| SO ₄ ²⁻ | 0.1 |
| Cl ⁻ | 0.1 |
| PH | 0.2 |
| TDS | 0.15 |

2.3 Geospatial Artificial Intelligence (GeoAI) for Groundwater Quality Simulation

In the modeling process, ANN, SOM, and CANFIS methods were used to simulate groundwater quality. Moreover, the same data were used for the training and test processes for each method. First, all data were divided into two splits: training data (60% for modeling and 10% for cross-validation), and test data (30% of the data). Data were normalized and the training process was performed. Then, the testing or validation was carried out and further the results were compared with the same statistical indices (R-sqr, MAE, and MSE). A sensitivity

Table 3 Factors affecting groundwater quality and GWQI index in some drinking water wells

| No | GWQI | Transmissivity (m ² /day) | Groundwater depth (m) | Elevation (m) | Distance from contaminant centers (m) | No. of household | Population (person) |
|----|--------|--------------------------------------|-----------------------|---------------|---------------------------------------|------------------|---------------------|
| 1 | 0.2715 | 1500 | 12.90 | 50 | 6.4 | 52 | 460 |
| 2 | 0.2401 | 750 | 3.00 | -11 | 153.8 | 239 | 1077 |
| 3 | 0.2267 | 175 | 5.00 | -13 | 99.4 | 32 | 144 |
| 4 | 0.2165 | 750 | 4.00 | -10 | 1121.2 | 21 | 98 |
| 5 | 0.2125 | 1500 | 5.00 | 11 | 0 | 22 | 93 |
| 6 | 0.2070 | 500 | 4.17 | 6 | 20 | 246 | 1105 |
| 7 | 0.1971 | 1000 | 5.00 | 11 | 0 | 22 | 93 |
| 8 | 0.1969 | 750 | 6.50 | 20 | 20 | 161 | 666 |
| 9 | 0.1553 | 500 | 31.00 | 1062 | 830 | 30 | 95 |
| 10 | 0.1483 | 300 | 23.00 | 453 | 1100 | 13 | 62 |
| 11 | 0.1252 | 300 | 25.00 | 69 | 709 | 53 | 287 |
| 12 | 0.0568 | 100 | 38.00 | 1670 | 1023 | 53 | 342 |
| 13 | 0.2578 | 500 | 4.70 | 6 | 44 | 109 | 495 |
| 14 | 0.2042 | 750 | 3.50 | -8 | 451 | 92 | 434 |
| 15 | 0.3413 | 3000 | 5.00 | 20 | 15.42 | 574 | 2770 |
| 16 | 0.3252 | 2000 | 3.00 | 2 | 66.37 | 118 | 820 |
| 17 | 0.3243 | 1000 | 1.00 | 3 | 28.07 | 239 | 1187 |
| 18 | 0.3146 | 1000 | 1.00 | 1 | 21.27 | 136 | 800 |
| 19 | 0.2597 | 750 | 5.00 | 12 | 9.21 | 607 | 2931 |
| 20 | 0.2571 | 1500 | 8.00 | 33 | 194.20 | 144 | 693 |

analysis of the model inputs was performed to select the main parameters of groundwater quality. Studying the effect of inputs on the outputs and determine the importance of each input. The results showed that the transmissivity of aquifer formations, groundwater depth, and distance from industrial areas were significant factors in determining the groundwater quality and are the best inputs in groundwater quality simulation. In the following, the methodology of each of the three methods is described.

2.3.1 Artificial Neural Network (ANN)

An ANN consists of three layers, an input layer, a hidden layer, and an output layer. A network can have more than one hidden layer. In this study, multi-layer perception (MLP) was used to simulate groundwater quality. The MLP was generated by adding one or more hidden layers to a one-layer perception, and this proposed topology can solve complex problems (Tokar and Marcos 2000). The determination of the network's best structure and the number of neurons is important in network planning. MLP is the most realistic neural network architecture for classification or regression problems based on the literature (Lim et al. 2000; McGarry et al. 2001; Cohen and Intrator 2002; Gholami et al. 2015a, b). A three-layer (input, hidden, and output) feed-forward neural network was used with different learning techniques to simulate the groundwater quality index (GWQI). The feed-forward neural network is the first and simplest of artificial neural networks devised. In the feed-forward network, the information moves in only one direction forward, from the input nodes, through the hidden nodes, and the output nodes.

The MLP network was trained and optimized by a trial- and- error method. The trail-and error approach is the most applied method to find the optimum structure and the learning technique (Isik et al. 2013). The goal of network training is to determine how the network can simulate the relation between inputs and output variables. The modeling process was executed by NeuroSolutions software. The numbers of hidden neurons was varied from 1 to 10. The Levenberg–Marquardt (LM) training technique was found to be the best learning technique in groundwater quality simulation. Network training is part of the main stages in modeling using ANN. In the training process, the weight coefficients were calculated in intermediate and output layers (Tokar and Marcos 2000; May et al. 2008; Castelletti et al. 2012). The ANN model structure's determination involves defining the number of layers, the number of nodes in each layer, and how they are linked (Isik et al. 2013). The trial–error method and sensitivity analysis selected the appropriate input parameters. Eight input patterns were examined, and their performance was compared (Eq. 2 to Eq. 9):

$$GWQI = cf(T, Gw, Lc) \quad (2)$$

$$GWQI = f(T, Gw, Lc) \quad (3)$$

$$GWQI = f(T, Gw, Lc, H) \quad (4)$$

$$GWQI = f(T, Gw, Lc, H, P) \quad (5)$$

$$GWQI = f(T, Gw, Lc, H, P, F) \quad (6)$$

$$GWQI = f(Gw, Lc, H, P, F) \quad (7)$$

$$GWQI = f(T, L_c, H, P, F) \quad (8)$$

$$GWQI = f(T, Gw, H, P, F) \quad (9)$$

where $GWQI$ is the groundwater quality index, T is the transmissivity of aquifer formations (m^2/day), Gw is the groundwater depth (m), and L_c is the distance of a well from contaminant and residential centers (m). P and F are populations, and the number of households in the area 1 km^2 and H is the elevation (m).

2.3.2 Co-Active Neuro-Fuzzy Inference System (CANFIS)

In this study, a neuro-fuzzy hybrid model was utilized as well. The neural-fuzzy network is a feed-forward network supervised by a neural network learning algorithm through back-propagation during network training. Here various input vectors and an output vector were utilized. In the design of the neuro-fuzzy hybrid model, a trial-and-error approach determined the structure of the optimized input. The difference between the rate of observed and simulated water quality index is the objective function and the goal is to equalize the simulated and observed values. The rate of instantaneous error will be equal to zero according to Eq. (10):

$$J_i(n) = t_i(n) - a_i(n) \quad (10)$$

where $J_i(n)$ is the network moment error and represents the total error for neuron i in the output layer. $t_i(n)$ represents the desired target output of the i th network in the n th iteration, and $a_i(n)$ represents the predicted output from the system and is the actual output at each iteration. The model's selected weight was modified by estimating the output error and application of the back-propagation process. Weight correction was done using a gradient descent method and according to Eq. (11):

$$W_{ij}(n+1) = w_{ij}(n) + \eta \delta_i(n) x_j(n) \quad (11)$$

where $W_{ij}(n+1)$ is the synaptic weight to the i th neuron in the output layer from the j th neuron in the previous layer. $w_{ij}(n)$ is the rate of the weight in n th iteration, n denotes the steps of the iteration. g is the extent of step size or the learning rate coefficient because of controls the speed (Loganathan and Girija 2013), $\delta_i(n)$ is the local error of the modeling. It has been estimated from $J_i(n)$ in n th iteration, $x_j(n)$ is the regressor vector, and $\delta_i(n)x_j(n)$ is the gradient vector of the performance surface at iteration (n) for the i th input node.

The modeling process included the separation of training data and test data, how to optimize, select the optimal network structure and test the network in all three methods were the same.

2.3.3 Self-Organizing Map (SOM)

SOMs, which are nonlinear time-series models, are among those supervised learning methods that are used for classification and regression (Vapnik 1998; Bahrami et al. 2016). SOMs find an optimized decision-making plan to separate two mentioned classes so that two classes have the highest margin of separation in binary classification. In the SOM

algorithm (Kohonen map), the dimensions of the data are cut through the self-organizing neural network application. This technique aims to reduce the dimensions of the data to one or two dimensions. In this method, the only known parameter is the input neurons, while the weight and output neurons are the unknown parameters that must be found. Further, each input vector $x \in R^n$ can be evaluated with the m_i ; R^n in any metric, usually the Euclidean distance (the length of a line segment between the two points). In fact, the SOM defines a mapping from the input data space R^n onto a regular two-dimensional array of nodes. The winning node c is then calculated by (Eqs. 12 & 13):

$$\|x - m_c\| = \min\{\|x - m_i\|\} \tag{12}$$

$$c = \operatorname{argmin}\{\|x - m_i\|\} \tag{13}$$

where x is mapped onto c relative to the parameter values m_i .

The updated formula is as follows (Eq. 14):

$$m_i(t + 1) = m_i(t) + h_{c,i}(t)[x(t) - m_i(t)] \tag{14}$$

where t is the discrete-time coordinate and $h_{c,i}$ is a function defining the neighborhood. The initial values of the m_i can be random (Kohonen et al. 1996).

2.4 Evaluation of ANN, SOM, and CANFIS Performances

In the training phase, the best inputs were determined by changing the pattern of data inputs and analyzing the ANN, CANFIS, and SOM sensitivity to input data. In the next step, each of the three models' optimum structure was selected by utilizing a trial-and-error approach and testing their performance and error criteria. The models' performance was evaluated by using the mean squared error (MSE) and the coefficient of determination (R-sqr), defined as (Eqs. 15 & 16):

$$MSE = \frac{\sum(Q_i - \hat{Q}_i)^2}{n} \tag{15}$$

$$R - \text{sqr} = \left[\frac{\sum_{i=1}^n (Q_i - \bar{Q}_i) \cdot (\hat{Q}_i - \bar{Q}_i)}{\sqrt{\sum_{i=1}^n (Q_i - \bar{Q}_i)^2 \cdot \sum_{i=1}^n (\hat{Q}_i - \bar{Q}_i)^2}} \right]^2 \tag{16}$$

where Q_i is the observed value, \hat{Q}_i is the simulated value, and \bar{Q}_i is the mean of the observed data and $\bar{\hat{Q}}_i$ is the mean of the simulated data and n is the number of data points.

Finally, the observed GWQI values and the simulated GWQI values were compared in the test stages of the three used methods. The results of the test stages and the error criteria values were used to evaluate the methods' performance and to select the best method for simulation of the groundwater quality.

2.5 Groundwater Quality Mapping

Based on the results, the fuzzy neural network has the best results in simulating groundwater quality, and needs three inputs (G_w , T_a , and D_{industry}). Therefore, the CANFIS network was coupled with GIS for the generation of a groundwater quality map. Raster layers corresponding to the three mentioned factors were prepared and were combined at a resolution of 50 by 50 m. One can use a higher spatial resolution which will lead to more accurate input values, e.g. the distance from the pollutant centers. In the CANFIS network environment using the tested optimal network, GWQI was estimated for ten thousands pixels. GWQI values of 85 studied drinking water wells were overlapped on the simulated raster layer of groundwater quality. The results' accuracy and precision were evaluated by comparing the simulated values of GWQI and the observed values of GWQI. The layer of groundwater quality was presented as a groundwater quality map after classification.

3 Results

3.1 Groundwater Quality Modeling

The groundwater quality index (GWQI) in 85 studied wells based on observational data ranged from 0.05 to 0.34 and the mean GWQI was estimated at 0.21. The mean groundwater depth varied from one meter in the coasts to 40 m in the south of the plain. The transmissivity of aquifer formations has a range between 75 m²/day in fine-grained formations to 3000 m²/day in light-textured structures. Distance from industries is an important and influential factor in groundwater quality, and ranged from 10 m to several kilometers in study wells. The correlation coefficient between the GWQI and the factors of distance from industries, the groundwater depth and transmissivity of aquifer formations was estimated to be -0.56, -0.68 and 0.55, respectively. Therefore these factors are the most important ones in the groundwater quality assessment in the study plain. There is an inverse relationship between groundwater quality and distance from industry, and the closer we get to industry, the larger the pollution (Gholami et al. 2015a, b). The transmissivity of aquifers is also directly related to the emission of pollutants (Shi et al. 2016). Moreover, the higher the groundwater depth, the greater the risk of contamination (Adamowski and Chan 2011; Gholami et al. 2015a, b). Other factors such as precipitation, population and site elevation did not have a strong significant relationship with the GWQI in the study plain.

The modeling process was performed using the same data and three methods to simulate the groundwater quality. Table 4 illustrates the results of the training stage (R-sqr and

Table 4 Results of network training for simulating GWQI among the three used models

| Model/criteria | R _{sqr} | MSE | Mean absolute Error | Min Abs error | Min ax Abs error |
|----------------|------------------|---------------|---------------------|---------------|------------------|
| ANN | 0.95 | 0.006 | 0.03 | 0.003 | 0.06 |
| CANFIS | 0.98 | 0.0004 | 0.018 | 0.001 | 0.05 |
| SOM | 0.96 | 0.0008 | 0.02 | 0.003 | 0.08 |

MSE). The cross-validation stage was performed for suitable training, and MSE values in the three applied methods were estimated from 0.008 to 0.02.

Table 5 shows the test stage results to evaluate the performance of three models in GWQI estimation. In the training stage of the ANN method, the mean square error (MSE) and the coefficient of determination (R-sqr) were 0.006 and 0.95, respectively. While, in the test stage, they were 0.005 and 0.73, respectively. The optimal ANN was a MLP network with two hidden neurons, the LM learning technique, and the tangent hyperbolic transfer function. In the training stage of the CANFIS method, the MSE and R-sqr were 0.0004 and 0.98, respectively. While, in the test stage, they were 0.004 and 0.89, respectively. In the training stage of the SOM method, it was revealed that the MSE and R-sqr are 0.0008 and 0.96, respectively. In the test stage, they were 0.008 and 0.8, respectively.

According to the results, the CANFIS method has the best results in groundwater quality modeling among the three applied methods. Figure 2 shows a comparison between the simulated values and the observed values of GWQI by using the three methods.

3.2 Groundwater Quality Mapping

Groundwater quality of the study plain using the predicted GWQI values by the tested CANFIS network and the GIS tool was simulated. After classification of the simulated GWQI, the groundwater quality map was presented in Fig. 3. Moreover, GWQI values of 85 drinking water wells were overlapped on the groundwater quality map to assess the accuracy and precision of the results by comparing the predicted values and the observed values. The classified GWQI map was used for evaluating the groundwater quality in the Mazandaran plain. According to the produced groundwater quality map, most of the study plain area has moderate groundwater quality and a limited part has very good groundwater quality or polluted groundwater quality.

4 Discussion

In the training stage, it was found that the best inputs include three inputs: groundwater depth, distance from the pollutant centers, and transmissivity of aquifer formations. The mentioned factors are the most important factor in groundwater quality in the study area (Gholami et al. 2015a, b; Sahour et al. 2020). According to the statistical analysis, these factors have the highest correlation with groundwater quality. The main issue in the modeling process is the selection and accuracy of inputs and output. The groundwater depth and transmissivity of aquifer formations were measured by Mazandaran regional water

Table 5 Results of network testing among the three used models

| Model/criteria | R _{sqr} | MSE | Mean absolute error | Min Abs error | Min ax Abs error |
|----------------|------------------|--------------|---------------------|---------------|------------------|
| ANN (MLP) | 0.73 | 0.005 | 0.04 | 0.003 | 0.06 |
| CANFIS | 0.89 | 0.004 | 0.02 | 0.001 | 0.05 |
| SOM | 0.8 | 0.008 | 0.03 | 0.004 | 0.07 |

Fig. 2 Comparison between the simulated and observed GWQI values in the validation (test) stage for three used methods **A** ANN (MLP) network **B** CANFIS network and **C** SOM method

company (MRWC). The distance from the pollutant centers can be measured using satellite images and GIS. Therefore, the models inputs are available.

The results showed that the ANN has a high performance in groundwater quality simulation. The ANN can be applied to simulate hydrologic variables in an extensive area. The results also showed that the MLP network produces the best performance for the LM learning technique and the tangent hyperbolic transfer function. Using ANN for hydrologic simulation followed good results in the past, and, in most cases, there has been a high correlation between simulated and observed values (Crawford and Linsley 1966; Chang et al. 2002).

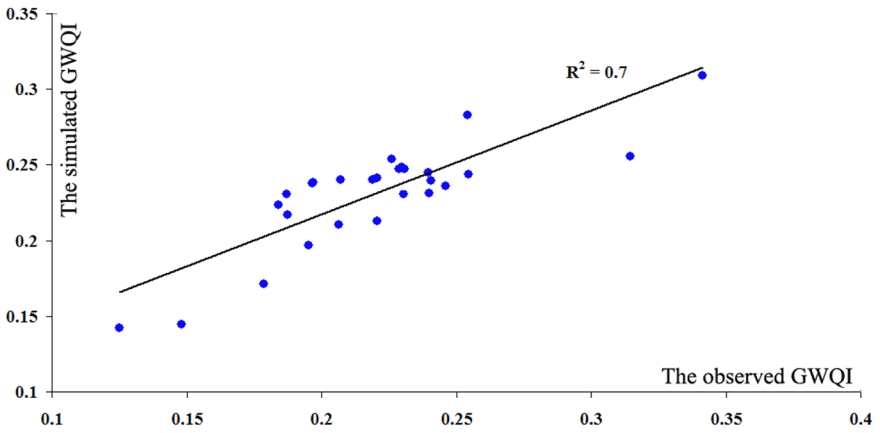
According to the results of Table 4 the results of the three models and associated GeoAI are acceptable and satisfactory in the training phase. The results showed that the SOM has an acceptable accuracy in estimating the GWQI index in the test stage.

The results of this study also indicated the acceptable ability of the CANFIS network in the simulation of groundwater quality. Previous research results showed high performance of the neuro-fuzzy network with the structure of the Takagi–Sugeno–Kang (TSK) model in estimation and hydrologic simulations as well (Jang et al. 1997; Talei et al. 2010; Heydari and Talaei 2011). The results of present study showed that the neuro-fuzzy network has a higher performance in estimating the groundwater quality index ($R\text{-sqr}=0.89$ in the test stage). Such results are consistent with the results of other researchers (Heydari and Talaei 2011; Allawi et al. 2018).

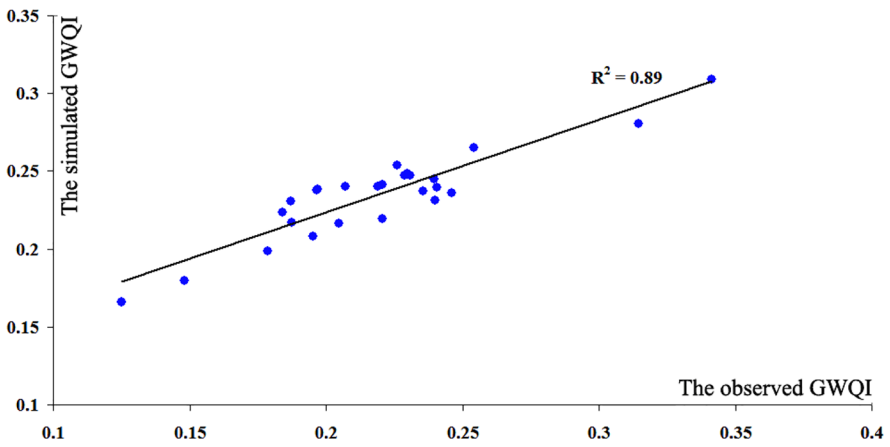
Comparing the observed and the estimated values of GWQI showed the performance of the used methods, and the high performance of the procedure of incorporating the applied methods to GIS (Krishna et al. 2008). All three methods of ANN, SOM, and CANFIS had acceptable accuracy in simulating the groundwater quality. But, the CANFIS method has the higher performance than the SOM and ANN methods. The maximum error in the simulation was observed in the minimum and maximum values of the GWQI. Models are generally more efficient in medium values and the maximum error in the modeling process is observed in the maximum and minimum data (Sahour et al. 2020). In the discussion of water quality, accurate estimation of maximum and minimum water quality index values is important to identify contaminated zones or zones with very good drinking water quality. Comparison of the results of the test phase has shown that the neural fuzzy method has the least error in modeling the maximum and minimum values compared to the other two methods, which is a potential for identifying contaminated zones with high accuracy. Finally, the method used to classify water quality in general or to achieve water quality classes have performed very well.

It is possible to estimate groundwater quality indices using artificial intelligence in a short period for sites without qualitative measurements. Therefore, the coupling of artificial intelligence and GIS is a promising way forward to support groundwater quality assessments and management. The groundwater quality map was generated by the coupling of CANFIS and GIS tools. Fortunately, the quantitative data of network inputs are available in the study area. Therefore, one can use the present methodology to model groundwater quality on the study plan's surface.

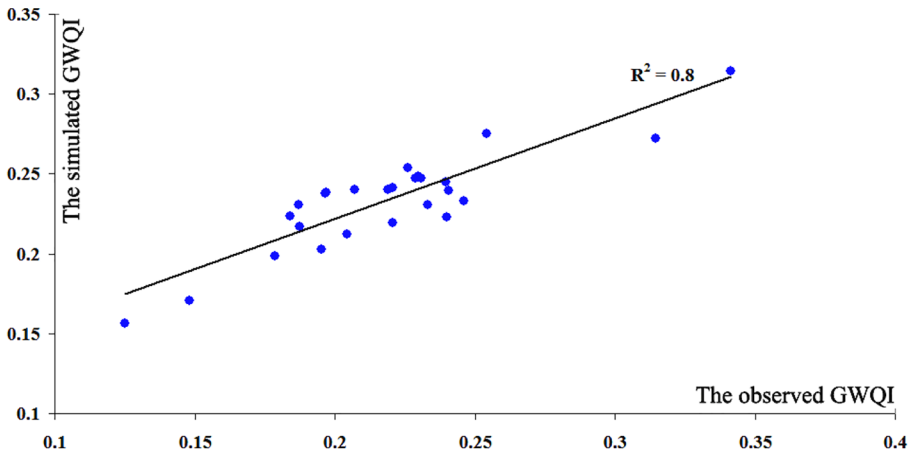
The produced groundwater quality map can be a tool for groundwater quality classification, planning water resources management, and their quality protection. Further, in the discussion of land management and the establishment of different industries and landuses,



(A)



(B)



(C)

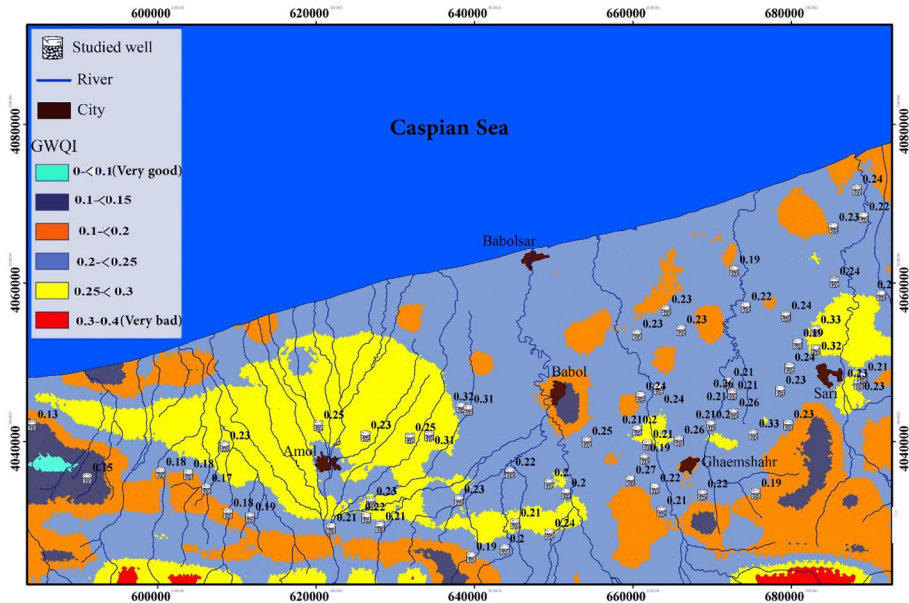


Fig. 3 Map of groundwater quality (GWQI) results from the coupled CANFIS network and GIS environment with a resolution of 50 by 50 m (the east of study plain). In this map, an evaluation of the accuracy of the results was done using a comparison between the simulated GWQI values and the observed GWQI values (overlapped values in the map)

the mentioned map can be used, for example, in places with high pollution, the establishment of new industries should be prevented. The artificial intelligence models used in the present study have their own advantages and disadvantages. These methods are more accurate than traditional methods such as regression method. It is also possible to define different management scenarios in the form of changing inputs for the model and evaluate their effect on the groundwater quality. For example, changes in industrial distances from a specific location or fluctuations in groundwater depth can be used for the tested model and their effect on water quality in the model can be evaluated. They also have the ability to provide multiple models with a variable number of inputs appropriate to the region (existing data) but their performance will be different. In addition to all the advantages mentioned, these models are black boxes and their use requires expertise in the field of artificial intelligence. Moreover, their combined use with a GIS is not as easy as the traditional methods such as regression methods. Considering all the above issues, their use is recommended for high performance and quick modelling in water resources studies.

5 Conclusion

The results show that all models have acceptable accuracy in predicting the groundwater quality, but the fuzzy neural network has the highest performance. This study's findings show that the groundwater quality assessed using the CANFIS model was in good agreement with experimental data. Hence, it can be concluded that CANFIS has successfully assessed the

groundwater quality. All of the applied methods can be used in hydrological or environmental modeling. Further, the coupled artificial intelligence methods and GIS can be used for zoning groundwater quality and as a tool for planning and managing water resources. Coupling artificial intelligence with GIS tools can provide practitioners with an easily interpretable water quality production map to manage these resources. The best groundwater modeling results were found by using the fuzzy neural network in Mazandaran Plain, but the other methods such as ANN or SOM may have better results in the other places. Therefore, it can be recommended to apply this proposed approach of combining three models in other geographical locations. It can be also concluded that GeoAI mapping performance depends on inputs and output data and the modeling process. Therefore, using different artificial intelligence machine learning algorithms for groundwater quality assessment in future studies was suggested. These models can be used to predict and map the groundwater quality in the other regions, but they need to be optimized and tested. However, It can be concluded that the result of this study has good potential to contribute to SDG-6 (clean water and sanitation), SDG-11 (sustainable city and communities), and SDG-13 (climate action).

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Declarations

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