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Estimation of the Spatial Distribution of the Groundwater Quality Using the Combined Method of Geostatistics_ Artificial Neural Networks (Case study: the Miandoab aquifer)

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Abstract
Recent research has revealed that the drought crisis, which was traditionally associated with central provinces, deserts, and hot and dry regions, has extended its impact to the plains of Lake Urmia, particularly the Miandoab plain. This area has experienced a significant decline in groundwater levels, leading to reduced quality. The study aimed to examine groundwater quality parameters, including TH, TDS, EC, pH, and SAR, using data collected by the regional water company of West Azerbaijan in 2002 and 2011. The statistical data from 2002 were processed using statistical and Kriging methods and stored in a 31×26 grid format in ArcGIS software. This data was saved as a text file and used in artificial neural network simulation. The findings demonstrated that the Multilayer Perceptron model with an M6 structure exhibited a correlation coefficient of 0.92. This result, along with a mean square error of 0.562, indicates the effectiveness of the model in simulating groundwater quality in the Mianodab Plain. Lastly, sensitivity analysis determined that chlorine, acidity, and phosphate had the greatest influence on the simulation and prediction of sodium adsorption rates.

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Introduction

Access to freshwater is considered the most essential human need throughout life. Freshwater, defined by its minimal salt content, finds its largest available reservoir on Earth in groundwater resources (Ardvani, 2006). Two percent of freshwater is trapped in polar ice, rendering it unusable in its current state, while the remaining one percent comprises freshwater obtained from groundwater sources (Askari, 2010). Groundwater, unlike surface water, remains relatively unaffected by sudden changes in temperature and seasonal precipitation, making it a more reliable source for industrial purposes (Zabihi et al., 2015). Groundwater resources have long been valued for their providing drinking water and supporting agricultural activities. They generally possess higher quality and experience less pollution than surface water, but their quality can be affected by a decrease in quantity or local human-induced contamination (Rizu and Muser, 2004). Assessing groundwater quality necessitates access to relevant data and information. Furthermore, choosing the appropriate method for monitoring and evaluating changes in groundwater quality is a crucial step in managing regional groundwater resources (Salehi and Zeini Wand, 2014). Due to the importance of groundwater quality and the significant expenses associated with monitoring systems, designing an optimal monitoring network and extracting relevant data becomes essential. Therefore, analysis of such data becomes necessary. The effectiveness of a groundwater quality monitoring system depends on various factors, including selecting the appropriate water quality index, determining sampling points, and establishing the frequency of sampling. However, direct sampling and laboratory or field measurements are often costly and time-consuming, limiting their practicality. Hence, there is a need for methods that can efficiently monitor large areas and examine changing processes (Nabi et al., 2016). Advancements in science have facilitated the use of new technologies, such as satellite data reception and processing, as well as the implementation of software and information processing systems. These technologies often reduce costs while improving the accuracy and speed of projects. Several algorithms exist for spatial interpolation, some relying on ground-based geometric methods. Modern methods are now employed to predict, locate, and understand the relationships between parameters affecting the estimation of groundwater level fluctuations (temporal and spatial) and water quality interactions. Computer technology advancements have made Mathematical models increasingly prevalent in recent decades. One such model is geostatistics and artificial neural networks (Moasheri, 2013). Geostatistics combines the geological sciences, statistics, and probabilistic methods.

Khattar et al. (2018) conducted a study on the impact of Electronic Conductivity (EC) and sodium absorption ratio (SAR) on relative hydraulic conductivity (Kr) and saturation (KS) in clay loam (C) and sandy loam (SCL) soils using grid-based artificial neural networks. According to the findings, KS decreased as SARw increased. SCL soil consistently showed higher KS than to C soil across all water quality categories. The impact of SARw on clay soil was minimal, likely due to its preexisting high salinity. While Kr responded similarly to both ECw and SARw, the microstructure of clay soil displayed greater sensitivity to water quality. This affected the soil structure more than SARw. To assess the application of artificial neural networks (ANNs) in estimating Ks and Kr, two types of ANNs (FFBP and CFBP) and two training algorithms (Levenberg-Marquardt and Bayesian regularization with a uniform thresholding strategy) were utilized, along with various threshold functions. Additionally, multiple linear regression was employed for Ks and Kr predictions. The CFBP network, trained with the LM algorithm and utilizing LOGSIG-LOGSIG-TANSIG threshold functions, demonstrated the highest performance with a topology of 1-4-5-4, achieving MAE and R2 values of 0.17161 and 0.9945, respectively. ANNs were found to be significantly more effective than regression methods in predicting Ks. In another study by Tiri et al. (2018), the quality of surface water in Algeria's Qued El-Hai Basin was assessed for drinking purposes using a fuzzy inference system. The analysis considered three stations and ten parameters (pH, TDS, Ca, Mg, Na, K, Cl, SO_4, SO_4, and HCO_3), highlighting the dominance of calcium and sulfate ions across all stations. TDS showed a strong positive relationship with SO_4 and HCO_3. Temporal variations in the parameters, except for K and Ca, were not significant based on an ANOVA test. The quality of surface water was evaluated using the FWQI index, which was found to be similar to the WQI index. The main factors influencing surface water quality were the interaction between water and stone and human activities. In a review by Maaroufpour et al. (2017), the spatial distribution of groundwater quality in Kasht, Bam, Narmashir, and Rahmat Abad plains (Kerman-Iran province) was investigated using software calculations, statistical methods, ANN models, and ANFIS models. Kriging and Cokriging statistical methods were compared to ANN models for predicting the distribution of groundwater electrical conductivity (EC). Analysis was conducted on data from 24 wells spanning the period of 2002-2011. The ANN model, specifically with a triple input model (longitude, latitude, and several months) or a quadratic input model (longitude, latitude, month number, and CL), yielded more accurate results with the lowest RMSE and MAE values and the highest R^2 value. The land-tested land-use method was employed to generate EC data for unobserved areas. In a study by Heidarzadeh (2017), an ANN model was utilized to predict groundwater quality in the Amol-Babol aquifer using data from 1987 to 2010. Sodium concentration was selected as the response variable due to its high levels for irrigation purposes. The choice of wells studied in the neural network was determined using a geographic information system (GIS) based on sodium zonation over 20 years, with three pH characteristics, electrical conductivity, and total hardness identified as the most suitable input variables. The findings revealed that by training the model with data from six well-controlled and highly precise wells, it was possible to estimate sodium concentration in three other wells. The optimal network configuration consisted of a two-layer network with Logsig-Tansig transfer functions, consisting of four neurons in the first layer and three neurons in the second layer. During the training and validation processes, determination coefficients (R2) of 0.99 and 0.98 were achieved, respectively, with a Root Mean Square error (RMSE) of 0.88.

Heidarzadeh (1977) analyzed the groundwater quality of Amol-Babol Plain and conducted sodium zoning using GIS. The results indicated a critical pollution status, primarily influenced by land use near industrial areas and populated cities. El Aflya (2002) employed GIS techniques to assess groundwater pollution in the Al Arish, Sinai, and Egypt regions. The study identified phosphate fertilizers, nitrate, pesticides, sewage, and salinity as potential sources of groundwater contamination. Molayee et al. (2006) utilized a combination of satellite imagery and a radial basis neural network model to estimate suspended sediment load concentration. The results indicated that the artificial neural network model with inputs of band 1 and flow rate yielded better results (RMSE=0.19) compared to regression (RMSE=0.21) and sediment curve (RMSE=0.29) methods. One notable advantage of artificial neural networks is their ability to approximate various types of functions, adapt and update themselves, exhibit stability, and ease of use, and reduce the need for a deep understanding of variable-function relationships. Recent advancements in intelligent modeling techniques have highlighted the superior performance of artificial neural networks (ANN) compared to other statistical models (Azari et al., 2008; Nouri et al., 2008). Moasheri et al. (2012) estimated the spatial distribution of sodium absorption ratio (SAR) values in the Birjand Plain using a combination of geomagnetic and artificial neural networks. The results demonstrated that this method was highly suitable for estimating the spatial distribution of SAR, which is an important groundwater quality parameter. Moasheri et al. (2012) investigated the impact of soil aging characteristics on the prediction of cation exchange capacity (CEC) using artificial neural networks in the Kahsh district of Khorasan. The results showed that artificial neural networks with a structure of M40 (R^2=1.57 and MSE=0.358) outperformed regression models (R^2=57.1 and MSE=0.789) in predicting CEC. Zare Abyaneh et al. (2013) utilized neural smart methods, including multilayer perceptron neural networks, radial basis functions, and fuzzy and neural-genetic functions, to estimate point values of station levels in the Hamedan-Bahar Plain. The estimates from each intelligent neural method were compared with Geostatistical kriging to estimate station levels in unmonitored locations. The accuracy of the estimation methods showed that the genetic neural method outperformed the multilayer perceptron, radial basis, and neuro-fuzzy methods, respectively. Moasheri et al. (2013) employed a geostatistical integration method, specifically artificial neural networks optimized with a genetic algorithm, to estimate the spatial distribution of groundwater quality parameters in Kashan Plain. The study focused on the spatial distribution of sodium, calcium, and magnesium parameters. The findings revealed that this method exhibited superior capability in estimating the spatial distribution of these parameters in Kashan Plain. Bait Darbeshi et al. (2013) compared numerical modeling, artificial intelligent methods, and ground statistics to estimate groundwater levels in Hamedan-Bahmard Plain. The study utilized the numerical code MODFLOW in GMS software, artificial neural networks, neuro-fuzzy methods, wavelet-wave methods, and ArcGIS geodata methods. The accuracy of the estimation methods, based on the lowest mean squared error, ranked as follows: neural wavelet, neuro-fuzzy, ground statistics and artificial neural networks. Sadiq et al. (2014) studied the temporal and spatial trends of groundwater quality parameters in Kashan Plain using land statistics and Schooler and Wilcox diagrams. They analyzed 12 years of data (2002-2013) and weighted the parameters based on their impact on water quality changes. The circular dragging method in statistical analysis exhibited a more acceptable performance based on the correlation coefficient. Yazdani et al. (2016) evaluated groundwater quality indices in Mashhad Plain using geostatistical techniques and GIS. The results and maps indicated inadequate groundwater quality conditions, particularly in terms of total dissolved solids (TDS) and total hardness (TH) indices in the southern parts of Mashhad. Basirani et al. (2016) investigated the spatial distribution of the SAR parameter in Torbat Jam-Fariman Plain using the Kriging-ANN model. The study analyzed the rate and trend of changes in groundwater quality parameters, including Cl, Na, Ca, Mg, SO_4, EC, pH, TH, SAR, and TDS, using data from the

Water and Wastewater Company of Torbat Jam-Fariman Plain collected between 1997 and 2014. The results indicated that the compilation of statistical models with artificial neural networks provided a cost-effective and time-saving approach for estimating SAR values compared to laboratory testing. Ahmadifar et al. (2016) applied GIS to zone the risk of groundwater pollution in Sarab Plain. Delkhoush et al. (2016) performed qualitative zoning of groundwater in Mokhtaran Plain, focusing on drinking water quality, and found that groundwater in the study area was classified as unfavorable based on drinking water standards.

Yazdani et al. (2016) evaluated groundwater quality indices in Mashhad Plain using geostatistical techniques and GIS. The results and maps indicated inadequate groundwater quality conditions, particularly in terms of total dissolved solids (TDS) and total hardness (TH) indices in the southern parts of Mashhad. Hence, artificial neural networks can utilize nonlinear relationships within data and generalize results to other datasets. The drying of wells in the Miandoab basin, primarily caused by a significant proportion of unpolluted agricultural wells, has led to a severe decline in groundwater levels. This water crisis has directly affected the agricultural sector in the region, resulting in the drying up of numerous wells. The situation highlights the urgent need for accurate management of the aquifer, considering the limited availability of these reserves and the presence of salts and minerals within them. The drying wells serve as a warning to both the public and officials, indicating an imminent crisis in one of the previously prosperous areas of Miandoab City. Each year, the groundwater levels of the aquifer are impacted, underscoring the importance of comprehensive studies to assess quantitative and qualitative changes. These studies are crucial for the effective management and planning of groundwater resources in the region.

Materials and Methods

Area of Study

The study area of Miandoab is located in the provinces of West Azerbaijan and East Azerbaijan (between 45° 15 ‘to 45° 53’ east longitude and 36° 52’ to 37° 15 ‘ north latitude) (Fig. 1) and the water resources trustee is the West Azerbaijan regional water company.

The study area in question encompasses a total land area of 4,308 Km^2, equivalent to 3.8% of the overall Lake Urmia catchment area. Within this expanse, 1,366 Km^2 is attributed to the plain, making it the largest plain within the Lake Urmia catchment area. The remaining 2,962.9 Km^2 comprise the elevated regions of the study area (Water Report, 2011). The expansive plain encompasses 93.3% of the total area and includes a free-flowing aquifer covering 1,256 Km^2. Groundwater extraction resources, documented in 2009 and 2011, consist of 22,469 wells with an annual discharge of 34.31 billion cubic meters, 88 pipelines discharging 1.65 MCM, and 131 spring outlets releasing 47.48 MCM annually. For the alluvial aquifer region of Miandoab Plain, there are 17,509 extracted groundwater sites and two quarries with an annual discharge of 280.279 MCM. Additionally, within the Miandoab plain, there are eight deep wells and 64 partially submerged wells, while at the elevated regions of the study area, there are three wells, four springs, and four wells within the quaternary strata (Report of Water Bulletin, 2011). The highest elevation within this area reaches approximately 3,500 meters, corresponding to the altitudinal ranges of the Mordavikha mountains that extend from the slopes of Mount Sahand. Conversely, the lowest point within the range lies around 1,270 meters above sea level. Noteworthy cities within this region include Miandoab and Melcan (refer to Figure 1).

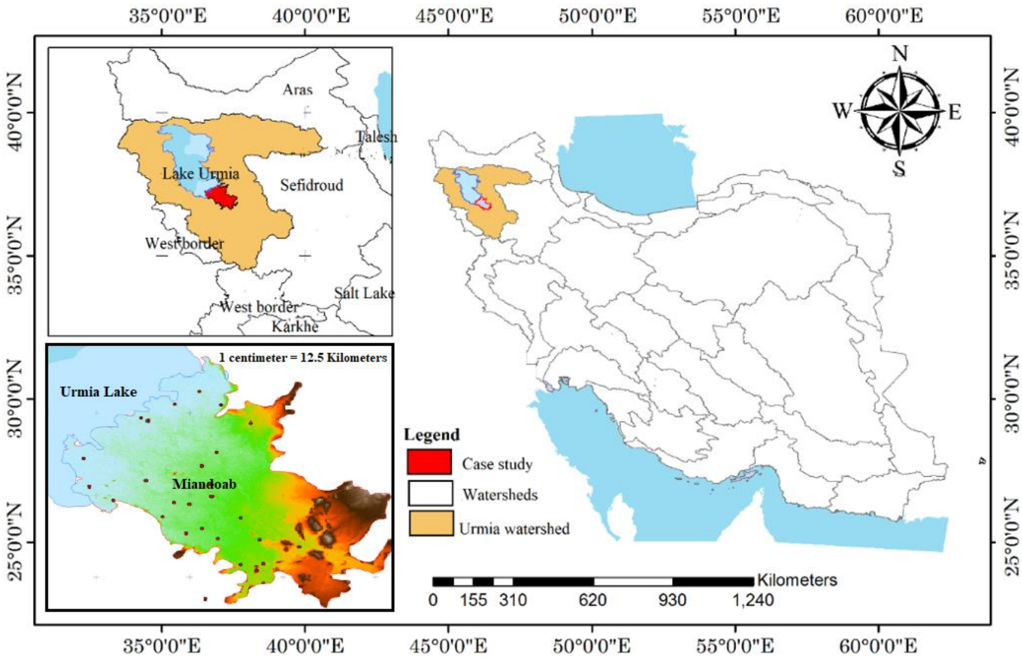

Figure 1. Location of the study area, Miandoab basin

Within the Miandoab study area, there are 24 stations, comprising one synoptic station, 10 rain stations under the supervision of the country's meteorological organization, 10 regular rain gauge stations, two evaporation stations, and one rainwater storage station operated by the Ministry of Energy. However, at present, four stations within this study area are inactive, while the remainder are operational. The temperature readings for the mountainous and plain areas are recorded as 9.4°C and 11.7°C, respectively. Rainfall serves as a crucial meteorological parameter and significantly contributes to the formation of water resources. The average annual precipitation is estimated to be 318.1 mm in elevated regions and 258.8 mm in plains. Ongoing studies focus on rivers within this range, including rivers with a length of 200 km and the primary Zarrinehrood river spanning 300 km (considered the most significant river within the Lake Urmia basin) (reported by Regional Water Company, 2011).

Regarding groundwater quality parameters, the study examined pH, EC, TDS, TH, SO_4, Cl, and SAR. Data for these parameters were collected from a total of 46 wells located in the Miandoab Plain area between 2002 and 2011 (refer to Figure 1). The regional water company of West Azerbaijan province facilitated the collection of these data. The objective of this research is to predict the spatial distribution of groundwater quality parameters within the Miandoab Plain using a statistical compilation method known as the artificial neural network. The obtained results will then be compared to the actual values for evaluation purposes.

Results and Discussion

The process of obtaining zoning maps and spatial distributions for groundwater quality parameters involves using ArcGIS 10.2.2 software. Skewness in the data is addressed by applying log-box or box-cox functions if necessary. The best model is selected based on visual analysis and the lowest error is determined by root mean square error. The optimal model size, number of lags, and neighbors are chosen iteratively to minimize error. Estimated values obtained through intersection and observed validation methods are stored in a regular n × m network. Statistical indicators such as MSE and R^2 are used to evaluate different methods, with cross-validation being an important technique for accuracy assessment. Artificial neural network modeling requires a substantial amount of data, so additional statistical methods are employed to generate more data when the available data is limited. Using GIS software, zoning maps, and spatial distributions are created for each qualitative parameter. A network is constructed based on the minimum well quality, and values of studied properties are extracted from the maps. Artificial neural networks are capable of accurately estimating complex functions with limited discontinuities. Input data selection is crucial, considering influential parameters and consistency in quantity between input and output data is important. Data preparation involves scaling or normalizing the data using the min-max function in MATLAB 7.6. In the grid design, feed-forward and feedback structures are used to determine the optimal number of hidden layers and neurons, with a genetic algorithm employed for optimization. The results are evaluated using statistical indicators like MSE and R.

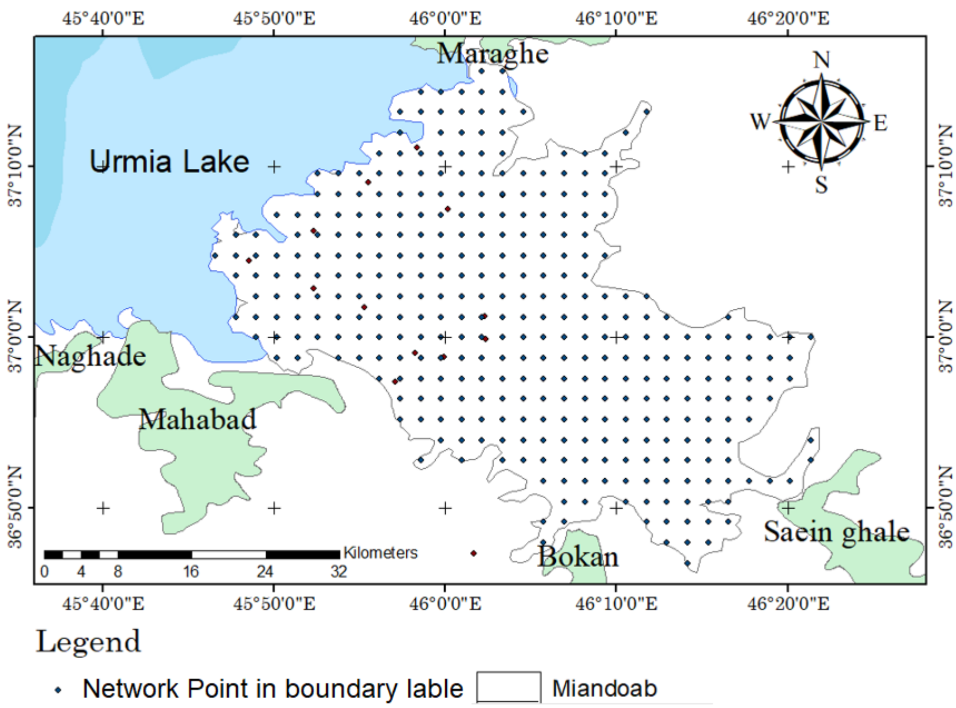

Figure 2. 26 * 31 grid for conversion of groundwater quality zones to textual and usable data in the artificial neural network.

Geostatistics

In simpler terms, spatial data exhibit a natural spatial property, which means that data points near each other are interconnected and not independent. Natural phenomena are interconnected and influenced by one another. When analyzing statistical patterns, there are several important considerations. These include the normality of the data, the presence of known trends or patterns, and the selection of an appropriate spatial model (Wackernagel, 1992).

The normality of the data is not a requirement for performing Kriging, a common spatial interpolation method. However, if the data distribution is non-Gaussian, classical Kriging methods may

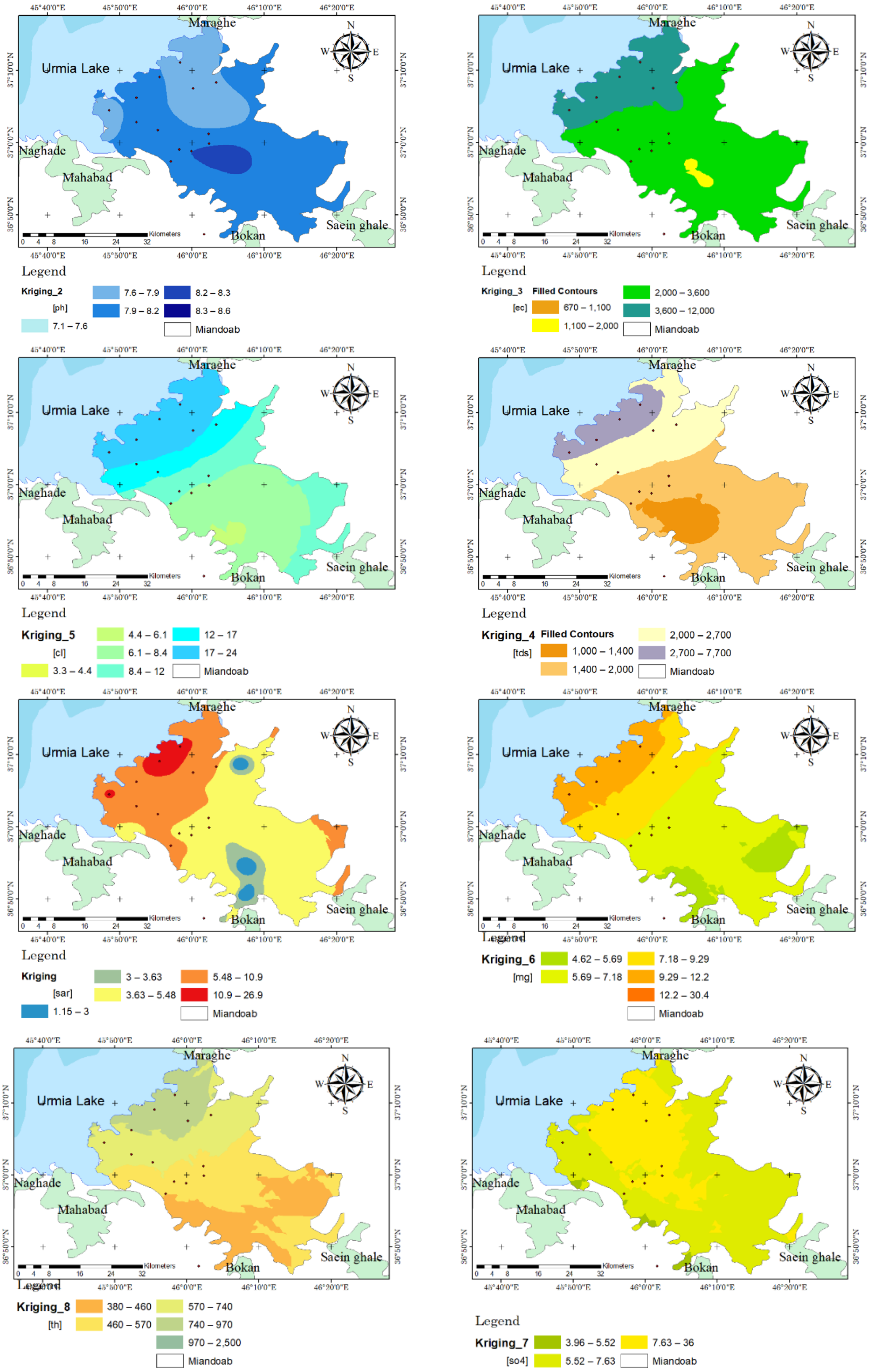

Figure 3. Spatial distribution maps of groundwater quality parameters of the Miandoab basin in 2002 by the Kriging method

not provide the most accurate estimates. Other factors that can impact the accuracy of spatial interpolation methods include the selection of an appropriate model and the presence of spatial trends within the data.

Artificial Neural Networks

Artificial neural networks were initially introduced in 1943 by McCulloch and Pitts, but their development was limited until the advent of computers and the introduction of the backpropagation algorithm by Ram Hart and Associates in 1986. This marked a significant advancement in the use of neural networks. Artificial neural networks are composed of interconnected elements that operate in parallel (Azimi et al., 2019). These elements are inspired by the structure of the human nervous system. By adjusting the communication values (weights) between the elements, an artificial neural network can be trained to perform specific tasks. This training involves comparing the network's output to a target output and adjusting the network based on the differences until the desired output is achieved. The overall structure of artificial neural networks is inspired by the biological network of the human brain.

The functioning of an artificial neural network can be summarized as follows (Moasheri, 2012):

1. Adjust the weights based on input-output pairs.
2. Initialize the weights with random values.
3. Load the training examples.
4. Calculate the network's output at the given inputs.
5. Modify the weights to minimize the difference between the output and the target.
6. Repeat the process for all training samples.
7. End the process when weight changes stabilize with minimal error.

To develop an artificial neural network model, various technical components need to be designed. Different network structures, such as the perceptron, are explored and their error values are determined to select and use the most suitable network (Khataar et al., 2018). Sensitivity analysis is used to understand the impact of factors involved in the simulation. The selection of an appropriate and optimal model is based on evaluation indices such as R (correlation coefficient) and MSE (mean square error). Before training the neural network, input data should be standardized to avoid issues with speed and accuracy. The standardization process ensures that data values are balanced, preventing excessive weight adjustments. Neural network models require three types of data: training, validation, and testing. Training data is used to establish the relationship between inputs and outputs, validation data are employed to monitor network learning and test data is used to evaluate the network's performance. NeuroSolution software is used for modeling artificial neural networks, which consist of input, hidden, and output layers. Normalized data within the range of [0, 1] is utilized to enhance accuracy and speed. Spatial distribution maps of groundwater qualitative properties are designed, and the required training data is generated using ArcGIS software. Finally, the significance of nonlinear correlations between parameters is determined using SPSS software, and the input parameters for the neural network simulation are selected based on the evaluation of parameter correlations.

Once the values of properties for each point in the 26 * 31 grid are determined, we utilize these values as training, validation, and test data for the neural network. Additionally, we employ the values from all sampling points as test data for the neural network. The data extracted from the 26 * 31 grid is divided into three subsets, with 60%, 15%, and 25% allocated for training, validation, and test data respectively. Based on Figure 4)), the inputs for the neural network are determined as total hardness, chlorine, sulfuric acid, acidity, salinity, and total soluble oils, while the output is set as SAR values (Fig. 5).

A10	A9	A8	A7	A6	A5	A4	A3	A2	A1	
									1	A1
								1	-.192**	A2
							1	.998**	-.188**	A3
						1	.872**	.867**	-.237**	A4
					1	.817**	.959**	.966**	-.166**	A5
				1	.843**	.832**	.951**	.936**	-.161**	A6
			1	-0.007	-.116**	-0.009	-.099**	-.101**	0.008	A7
		1	0.042	-0.033	-0.005	.166**	-0.006	-0.002	-0.003	A8
	1	-0.04	-0.002	.923**	.956**	.776**	.984**	.984**	-.160**	A9
1	0.007	-0.056	-.077*	0.004	0.001	.534**	.502**	.495**	-0.007	A10
*. Correlation is significant at the 0.05 level (2-tailed).										
**. Correlation is significant at the 0.01 level (2-tailed)										
K	SAR	HCO3	CO3	SO4	Cl	TH	TDS	EC	pH	Parameters
A10	A9	A8	A7	A6	A5	A4	A3	A2	A1	

Figure 4. Nonlinear Correlations of Quality Parameters of Groundwater of the iandoab Aquifer

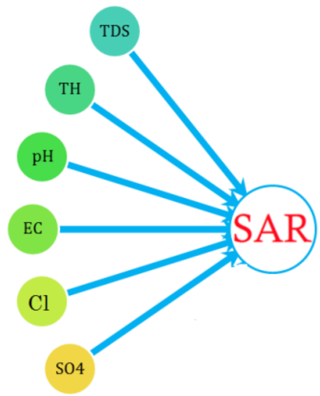

Figure 5. View the input layer and the output layer of the neural network

Once the inputs and the number of parameters for the network were determined, the next step involved designing the architecture of the neural network. Various GFF and MLP neural networks were implemented, considering different transfer functions and numbers of hidden layers. These networks were trained and tested to evaluate their performance. The results demonstrated that the MLP network with a single hidden layer, employing the Tan axon transfer function, achieved a high coefficient of reliability with R=0.96 and MSE=0.562, as shown in Table (1). This correlation coefficient serves as evidence of the neural network's capability to establish effective communication between inputs and their corresponding outputs.

According to the results of the analysis, there is a high correlation between the statistical parameters of the mean square error and the correlation coefficient between the values simulated by the neural network and the production data from the land statistics method (Fig. 6), and these components indicate the capability The superior artificial neural network is

in simulating and adjusting the quality parameters of the groundwater resources of the Miandoab aquifer.
As shown in Figure (6), there is a high correlation between the values simulated by the neural network and the data generated by the Geostatistic method.

Table 1. Analytical results of artificial neural network in estimating SAR values with all parameters

Performance	SAR
MSE	0.562
MAE	0.473
R^2	0.92

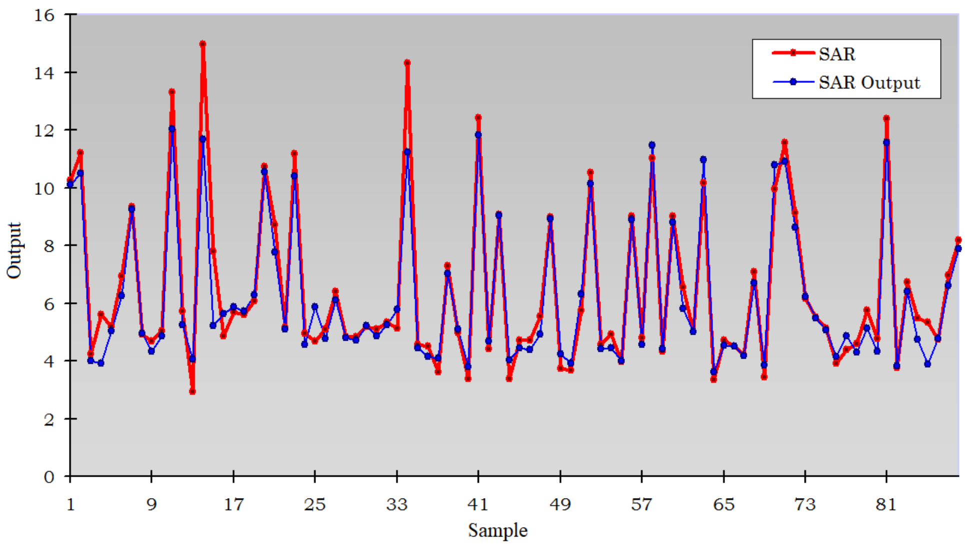

Figure 6. Correlation diagram of SAR values simulated by artificial neural network model and actual values sampled from wells in 200

Given this ability to predict sodium absorption ratios between 2003 and 2011, prediction results were compared with data from wells during this period.
The analysis of the results (Table 2) also confirms the efficiency of the artificial neural network in the prediction part, so the relative correlation between the predicted sodium absorption rate and the artificial neural network and the actual values obtained from the well sampling is illustrated in Figure (7).
Determination of the effect of each input parameter introduced into the neural network on the determination and prediction of SAR values was determined by sensitivity analysis (Figure 8). It was determined that chlorine, acidity, and phosphate values had the greatest effect on the simulation and prediction of the ratio of absorbed sodium.

Conclusion

This study utilized the Kriging-ANN model to analyze the spatial distribution of the SAR (Sodium Adsorption Ratio) parameter. The research found that by using a statistical model compilation approach combined with artificial neural networks, and utilizing easily obtainable data such as pH, EC (Electrical Conductivity), TDS (Total Dissolved Solids), TH (Total Hardness), SO_4 (Sulfate), and Cl (Chloride), it is possible to obtain a simpler and more cost-effective alternative to laboratory testing for determining SAR values in the Miandoab aquifer. Traditional methods of determining SAR values typically involve extensive time, cost, and significant safety measures. However, the findings

Table 2. Analytical results of artificial neural network in predicting SAR values between 2003 and 2011

Performance	SAR
MSE	4.094
MAE	1.635
R^2	0.69

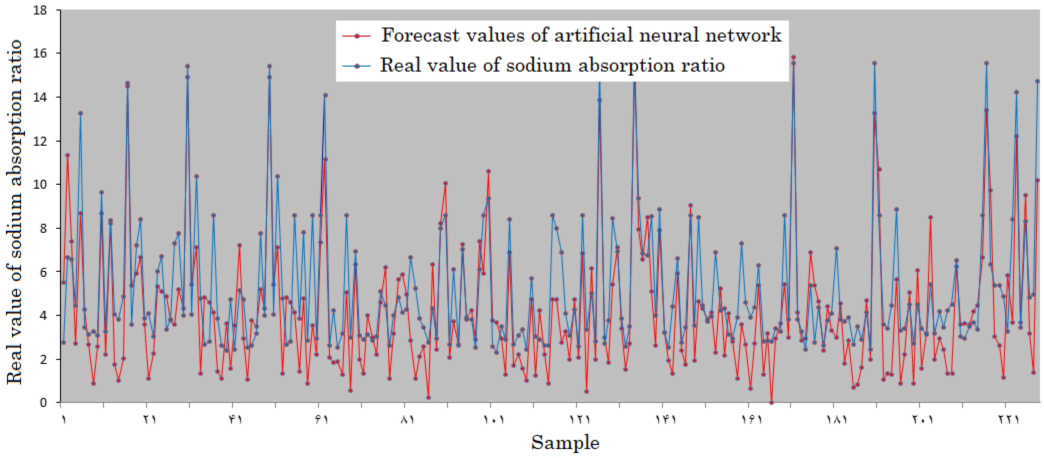

Figure 7. Correlation diagram of actual SAR values and predicted values by the neural network in 2003-2003

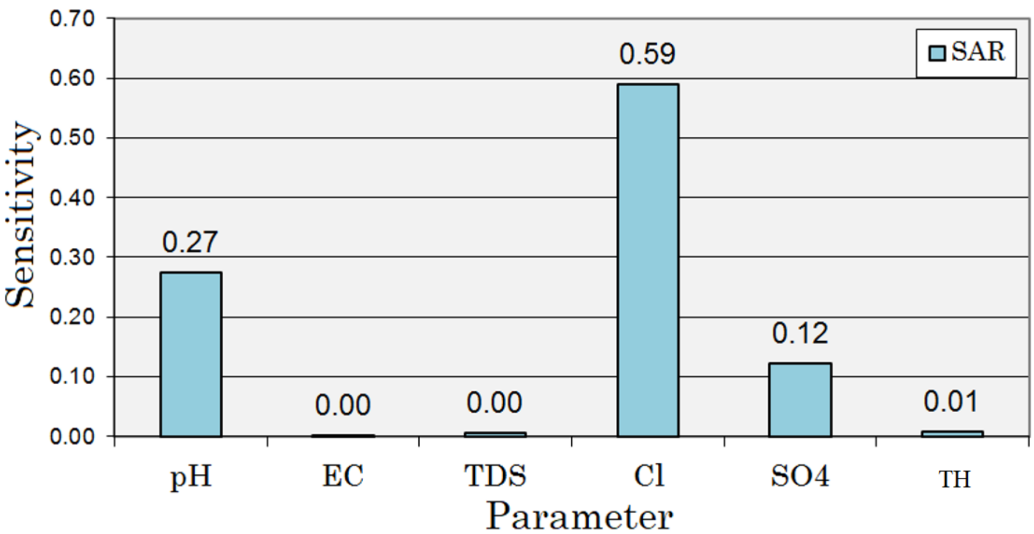

Figure 8. Sensitivity analysis

of this study suggest that the proposed approach offers a viable alternative that is less resource-intensive. By incorporating chlorine levels, acidity, and groundwater phosphate in the Miandoab plain, the sensitivity test results demonstrated that it is possible to estimate sodium admixture ratios with an approximate accuracy of 92%. Furthermore, the study also found that the rate of change in the sodium absorbance ratio over time can be estimated with a coefficient of approximately 69%. This information can be valuable for monitoring and predicting the variations in sodium absorption in the Miandoab aquifer over time.

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