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Groundwater Nitrate Modeling in Tehran Metropolis Using Artificial Neural Network and Kriging Methods

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Abstract

This study examined the relationship between groundwater quality and land use in Tehran. For this purpose, the possible relationship between the types of land uses and the concentration of nitrate in groundwater parameters was modelled using a Multi-Layer Perceptron (MLP) artificial neural network in geographic information system (GIS). The optimal network model was selected based on the mean root mean square error (RMSE) and correlation coefficient. Interpolation through Kriging was also performed to compare its results with those of the predicted model derived from an artificial neural network. The results showed that the neural network has a high capability for predicting and modelling groundwater nitrate concentration compared to the Kriging method. The high accuracy (RMSE: 0.003) of the neural network makes it a useful tool in relevant management issues. Our results of network sensitivity analysis were similar to scientific findings regarding the factors influencing the formation of nitrate in groundwater. Model outputs in the form of maps, tables, and graphs allowed the study of the role of each variable and the extent of its impact on groundwater quality. Performing various simulations and modelling of groundwater pollution provides an effective benchmark towards optimizing the management, control, planning, and decision-making in urban areas and can lead to economic and environmental savings.

1. Introduction

Groundwater provides about half of the world's drinking water and more than a third of the water used for irrigation (Smith et al., 2020). Groundwater quality is crucial in its protection and sustainability (Pandey et al., 2020). Public concern about groundwater quality has increased significantly in recent years due to inadequate surface water. In general, changes in land use patterns, climate, urbanisation, and population have led to a serious threat to groundwater quality (Kumar et al., 2017; Sharma et al., 2003; Wagh et al., 2018). Nitrate is one of the most common chemical contaminants in groundwater (Yu et al., 2020). Nitrate is an environmental pollutant that not only exists naturally but is also released by human activities, such as the production and use of fertilisers, combustion of fossil fuels, leakage and discharge of industrial and domestic wastewater systems, and change of natural vegetation by nitrogen fixation of crops (Gutiérrez et al., 2018; Torres-Martínez et al., 2021; Ward et al., 2018).

Nitrate is highly soluble in water and can gradually accumulate in groundwater systems (Gardner et al., 2020; Zhai et al., 2017). Therefore, increasing nitrate is a serious problem that affects the quality of groundwater in the region (Zhang et al., 2021). Various studies have been conducted on the factors that influence the level of

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nitrate in groundwater. Wang et al. (2020) investigated the parameters influencing nitrogen and nitrate levels in groundwater due to wastewater reuse. Natural elements such as land shape, soil type, and soil structure were examined, as well as human factors such as nitrogen fertiliser application, wastewater, land use, and land planting methods. Their findings revealed that the levels of nitrogen-nitrate in groundwater of different land uses varied depending on the type of human usage.

Similarly, Wu et al. (2021) discovered that groundwater in urban areas had much greater nitrate-nitrogen levels than in agricultural areas. According to Ransom et al. (2022), agricultural activities are a major contributor to elevated nitrate concentrations. El Amri et al. (2022) emphasised a substantial relationship between land usage and groundwater nitrate levels. They discovered that some land practices, such as forest maintenance, helped lower nitrate levels, but others, such as horticulture crop cultivation, tended to raise them (Cameron et al., 2013). Kim et al. (2021) also point out that groundwater quality will decline over the next few decades based on the age of the groundwater, the increase in nitrogen production from livestock activity, and the effect of nitrogen damping. Therefore, livestock land use can affect the amount of nitrogen in groundwater. The results of the study by Wang et al. (2020) also showed that nitrogen pollution is high in cities and agricultural areas, which indicates that nitrogen inflow from artificial sources is the main cause of groundwater pollution to nitrogen in their study area.

Based on previous research, there appears to be a direct relationship between nitrate concentrations and land use types. Consequently, this study investigates the relationship between groundwater nitrate levels and environmental parameters, aiming to draw a nitrate prediction map for the study area's metropolitan groundwater.To achieve this, nitrate modelling will be employed to illustrate how natural groundwater systems are affected by nitrate pollution. Since the performance of the neural networks in spatial prediction of pollution rate is weaker than the kriging method, they remain a strong competitor. Thus, this study will compare the effectiveness of two metropolis-scale approaches—artificial neural networks and kriging—in modelling groundwater nitrate levels.

2. Data and Methods

2.1. *Study Area*

The study area encompasses the Tehran Plain aquifer and the city of Tehran. Geographically, it is located approximately between latitude 35.715298°N and longitude 51.404343°E and covers an area of around 614 square kilometres. Tehran, the capital of Iran with a population of more than 12 million, began using its subsurface resources in 1963 (Karimi et al., 2019). With increasing population and rapid developments in agriculture and industry, groundwater exploitation has also increased significantly. Today, a significant part of the city depends on groundwater as the main source of water for irrigation of green spaces, gardens, and farms, which are supplied from wells dug inside and outside the city (Karimi et al., 2019).

According to the reports of Iran Water Resources Management Company, as a result of pressure on the city's groundwater resources, the annual water level has decreased by approximately 1.5 meters. In addition to the uncontrolled discharge of groundwater, the use of septic tanks in most areas of the city for wastewater disposal, development of agricultural lands and landfills, and the establishment of various industries, such as Tehran Oil Refinery in southern Tehran, have had major effects on groundwater quality. In terms of groundwater quality, due to the north-south slope in Tehran, in case of rain events, the final destination of all pollutants washed from the ground will be south of the city (Ghahremanzadeh et al., 2018). Figure 1 illustrates the geographical location of the study area.

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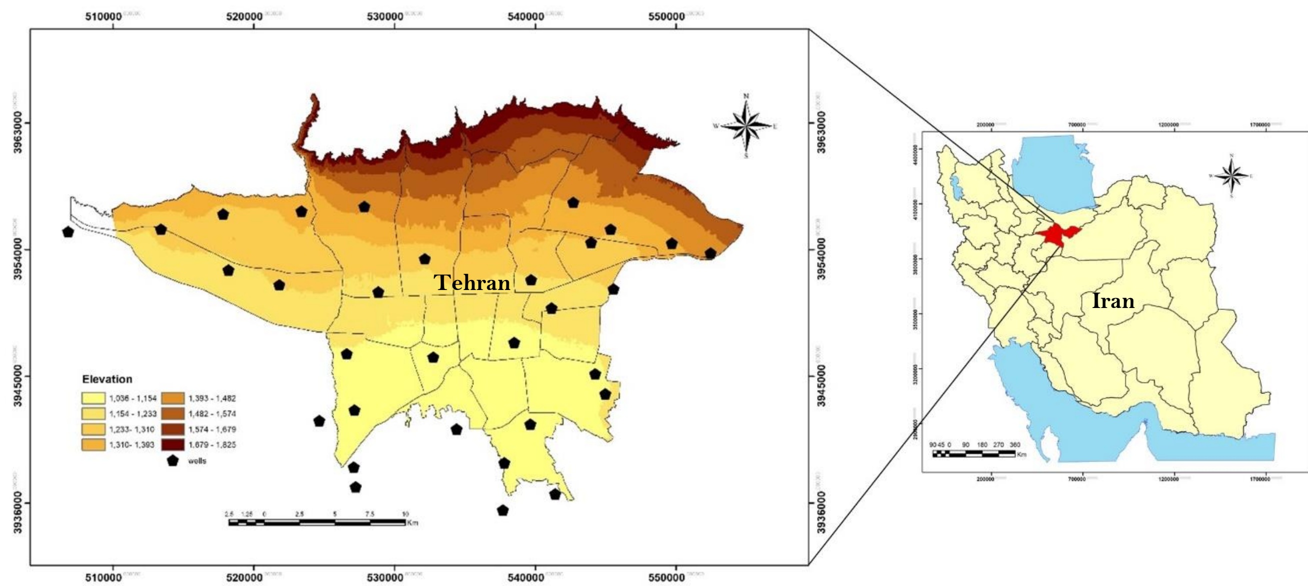

Figure 1. Location of the Study Area and Sampling Wells

2.2. Methodology and Data Sources

In this study, climatic, hydrological, and land use factors were used to achieve the effects of surface land uses in Tehran on groundwater quality. First, the factors affecting groundwater pollution were identified and selected. In the second stage, by collecting statistics, data, and information about the quality of wells and analysing them using the neural network, the effects of land use on groundwater quality were evaluated and simulated. Figure 2 explains the research flow

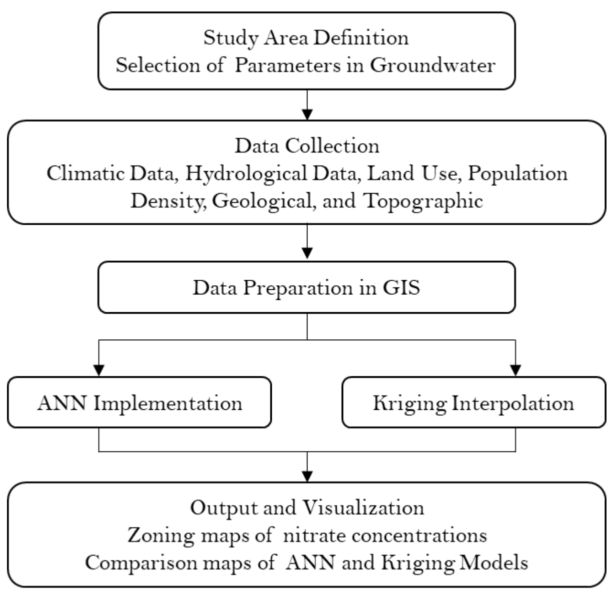

Figure 2. Methodology Framework

2.2.1.Preparation of Input and Output Data to the Neural Network9

All data used in GIS must be geometrically consistent and must also follow a single coordinate system (ESRI, 2021). Therefore, in order to unify all the data in the studies of this research, a system of geographical coordinates and a single cell size was defined for all data so that the data are geometrically compatible. Therefore, to equalize the cell size of all raster layers, it was selected according to Table 1.

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Table 1. Geographical Characteristics of Spatial Data used in Neural Network

Type	Description
Min X	509456.75
Max X	554796.75
Min Y	3936167
Max Y	3964872
Number of columns	1511
Number of rows	957
Resolution	30 m
Coordinate system	UTM –ZONE 39 N
Reference unit	Meter

Variables affecting groundwater quality when using Multi-Layer Perceptron (MLP) Neural Network and output are known as model nodes. In the MLP model, each input layer node is associated with all hidden layer nodes and each hidden layer node is associated with only the output layer node. The nodes and variables of each node are listed in Table 2.

Table 2. Data used in MLP neural network

Variable Name (Node)	Layer type
Distance from vegetation	
Distance from permanent and seasonal rivers	
Distance from main streets and highways	
Digital elevation model	
Slope	Input
Geology	
population density	
Water table	
Precipitation data	
Nitrate	Output

2.2.2. Data Preparation in Artificial Neural Network Modeling in GIS

The data used in artificial neural network modeling can be divided into two types, namely independent variables and dependent variables. for more details can be seen in the following explanation:

A. Independent Variables

Land Use Layer - For land use, the map prepared from the satellite imagery of Tehran (Available through Tehran Municipality based on 1 meter Ikonos images) in 1984 was used. Various derivative layers from the original land use map including pasture, agriculture, arboriculture, vineyards, parks, gardens, forests and grasses, permanent and seasonal rivers (canals), main streets and highways, as independent variables were derived in Shape format in the GIS environment. All vector layers were transformed into raster and then the distance on relevant layers was created using the DISTANCE module (Mihi & Benaradj, 2022) for later use in the model. Distance analysis was applied to vegetation, permanent and seasonal rivers and the main streets and highways.

Digital Elevation Model and Slope - From the topographic map with a scale of 1.25000 of the National Cartographic Center of Iran, using digital curve lines, a digital elevation model with a pixel size of 30 meters was prepared. The digital elevation model can be considered as a simple digital map that contains the altitude of all parts of the area covered. Also, the slope layer of the study area was prepared using the interpolated digital elevation model.

Geology - Using the 1: 100000 geological map of the Geological Survey and Mineral Exploration of Iran, a geological vector layer comprising sevenlayers (alluvium, young alluvial sediments, fine-grained sediments, bedrock, Kahrizak Formation, Hezar Dareh Formation) was prepared in the GIS environment.

Population Density - The population density variable was generated in the GIS environment using demographic data from Tehran, obtained separately from statistical blocks, and then the population density in each statistical block was calculated in terms of people per hectare.

Precipitation and water table data - In order to study the changes and the amount of rainfall in the region, monthly precipitation data of five synoptic stations including Tajrish, Mehrabad, Abali, Chitgar, Karaj and two climatological stations of Aminabad and Mamazan were prepared from the Iran Meteorological Organization (Table 3). Data was in Excel software format which was then spatialized in the GIS environment. In the next step, using precipitation data, interpolation was performed by Kriging method with a pixel size of 30 meters.

Table 3. Location of meteorological stations in Tehran

Station name	Station type	Latitude	Longitude	Height
Tajrish	Synoptic	35° 47´	51° 37´	1548
Mehrabad	Synoptic	35° 41´	51° 19´	1190
Abali	Synoptic	35° 45´	51° 53´	2465
Karaj	Synoptic	35° 55´	50° 54´	1312
Chitgar	Synoptic	35° 44´	51° 10´	1305
Aminabad	Climatology	35° 35´	51° 28´	1000
Mamazan	Climatology	35° 28´	51° 41´	1021

Source: Iran Meteorological Organization

All the above steps were performed for the water table level of piezometric wells obtained from the Regional Water Company of Tehran.

B. Dependent Variable

Nitrate - In this study, statistical information on the amount of nitrate related to 30 piezometric wells of the 2006 statistical year of the regional water company of Tehran was used for calculations. First, in Excel software environment, all data were classified separately for different years, and then in the GIS, the location of piezometric wells on the map was determined using the geographical coordinates of the wells and the location map of the piezometric wells was prepared. A 100-meter buffer was created around each point of the piezometric well.

2.3. Implementation of Artificial Neural Network

The initial raster data layers that were prepared in the raster format were changed to the desired format using the Export module and entered. In the next step, after determining nine input parameters and one output parameter to construct and determine the optimal architecture of the model, the input data was divided into three parts: the first part contains 60% of the data for training, the second part contains 20% of the data for authentication and the third part contained 20% of the data for the test.

During the artificial neural network training process, with increasing the number of iterations, the model error in predicting the training stage data is reduced to the point that in high iterations, the network is trained in such a way that it can only estimate the training stage data well and unable to predict data outside this range. In order to control this problem, a percentage of the data at the beginning of the work is considered for the authentication stage. By doing this, in each iteration, the amount of error related to the authentication stage is calculated simultaneously with the training stage. When the downward trend of this error rate is stopped, the model automatically completes the training phase and uses the previous iteration weights as the optimal model weights.

According to research, 90% of artificial neural networks used in hydrological problems are multilayer perceptron networks with post-diffusion algorithm. Therefore, to predict the concentration of nitrate in groundwater, a multilayer perceptron network was implemented with post-diffusion algorithm and hyperbolic and sigmoid tangent stimulation functions. One of the most important parts in the design of an artificial neural network is its architecture, or in other words, the number of hidden layers and the number of neurons in it, which is done by trial and error. Based on this, networks with different number of hidden layers and number of neurons in each layer were designed and their results were investigated and compared.

The network selected in the previous steps is used for training in this step. At the end of each training, the RMS and R2 error rates are determined and corrected by the BP training function among the distribution network nodes and network weights that were randomly selected at the beginning of the work. This is done as long as the RMS error is kept to a minimum. In the MLP model, it is possible to perform network training with long cycles. Of course, due to the time consuming performance of this number of cycles, it is practically not possible. Therefore, the network is trained to an acceptable number for modeling where the RMS error is kept constant at a low level. It should be noted that first, to train the network, the data of each factor was selected in a 100-meter buffer and the network was trained with this data. After performing this step and applying the required tests to validate the training output, the optimal model was selected. Considering that in the previous stage, the best possible network for the aquifer of Tehran was trained to predict nitrate concentration and its accuracy was measured based on the minimum root size of its RMSE and correlation coefficient, the sensitivity of the model outputs to the amount of nitrate is investigated.

To determine the effect of each of the independent variables on the model and finally on the amount of groundwater nitrate studied in the region, a sensitivity analysis was applied. At this stage, the data of the entire study space were entered into the network for prediction and were implemented using the optimal model selected from the training stage for the entire network area. This means that the network was implemented using the previous step training. All these steps for the amount of nitrate in groundwater were performed separately and the prediction results of each parameter were imported into Idrisi.

2.4. The Reason for Choosing the Multilayer Perceptron Neural Network

The multilayer perceptron neural networks developed by Rumelhart et al. (1986) and Shinde & Shah (2018) are among the most widely used neural networks (Taud & Mas, 2018). MLP consists of three layers: input, hidden and output. Due to the three-layer nature of this type of network, it is possible to identify nonlinear connections in nature.

2.5. Kriging interpolation method

The use of interpolation methods requires the existence of spatial architecture among the data, which is examined by variogram analysis. The condition for using this analysis is the normality of the studied data. The normal distribution of the sampled points results in better kriging performance in producing the predicted surface. The cations, anions and bicarbonate ions used in this study were first normalized using a geo-statistical analyst in the GIS environment through the histogram module and the Normal QQ Plot. In the next step, in order to create a model of groundwater nitrate parameter in Tehran, according to the sampled data of nitrate parameter, interpolation by kriging method was performed with a cell size of 30 meters in GIS environment and zoning map of each parameter was prepared for the desired year.

2.6. Comparison of Models

All interpolation maps generated to calculate the average in ASCII format were entered into the GIS. Using the Extract module, the average of prediction maps of the kriging model was drawn and the neural network prediction was calculated according to the 22 zoning of Tehran. Then, t-student-test was used to compare the two models. The second comparison using the VALIDATE statistical analysis module was used to compare the proximity of the prediction maps with the kriging model and the artificial neural network in the GIS. To perform statistical analysis of VALIDATE, the format of each of the above variables is converted to the format used in VALIDATE, which is the same as Byte Binary, using the linear expansion method, and its value range changes to the range of 0-255. This change of format is to unify the different data used in the model, which have different value ranges due to differences in their nature. Therefore, using the linear expansion method causes all the values in the independent variables to be expanded to the range of 0-255 and ready to perform the analysis. Then, using VALIDATE statistical analysis, the relationship between the two models was calculated.

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3. Result and Discussion

3.1 Predicting the Relationship between Independent and Dependent Variables

At this stage, an artificial neural network was implemented to study the effects of the status of independent input parameters including rainfall, population density, digital elevation model, geology, water level of piezometric wells, distance from vegetation, distance from main streets, distance from river and slope on the nitrate dependent parameter and the following results were obtained. Areas where the concentration of the dependent parameter is most predicted are shown more prominently in the map (Figure 3).

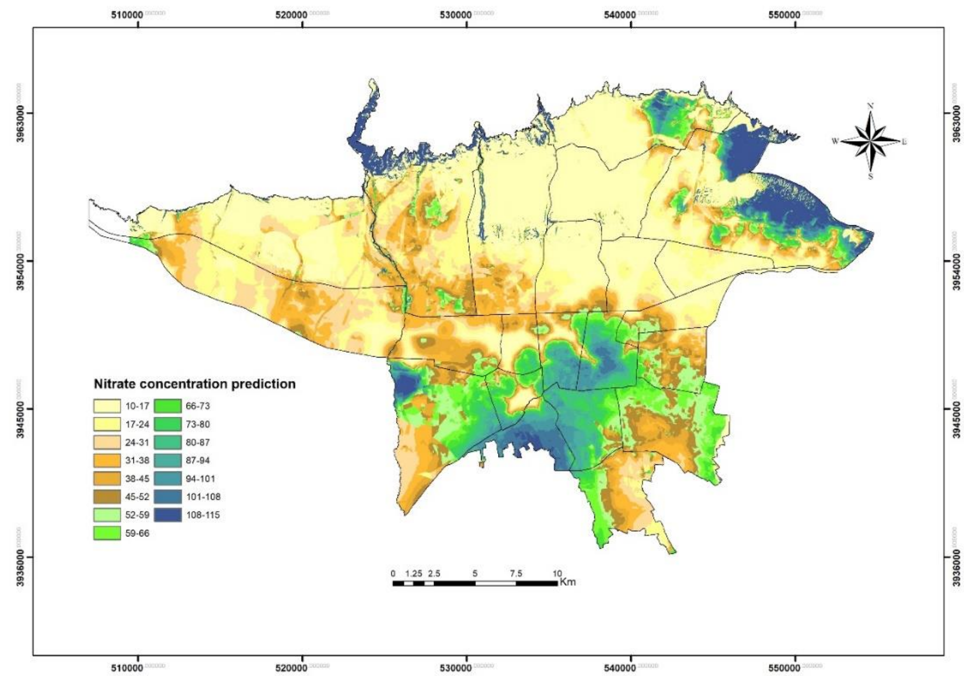

Figure 3. Map of Nitrate Ion Concentration Predicted by Neural Network Model

The artificial neural network MLP was implemented with nine input layers and one output layer for nitrate content. The criterion for selecting the optimal network model was the minimum root mean square error (RMSE) and the correlation coefficient and the model with the lowest error in comparing these two values was selected as the optimal model. The criteria for evaluating and selecting the optimal model are given in Table 4.

Table 4. Evaluation Criteria and Model Selection in Nitrate Ion

Network type	RMSE	R^2	Stimulus functions of output layer	Stimulus functions of hidden layer	Network layout
Perceptron	0.0033	0.99	Hyperbolic tangent	Hyperbolic tangent	9-7-1

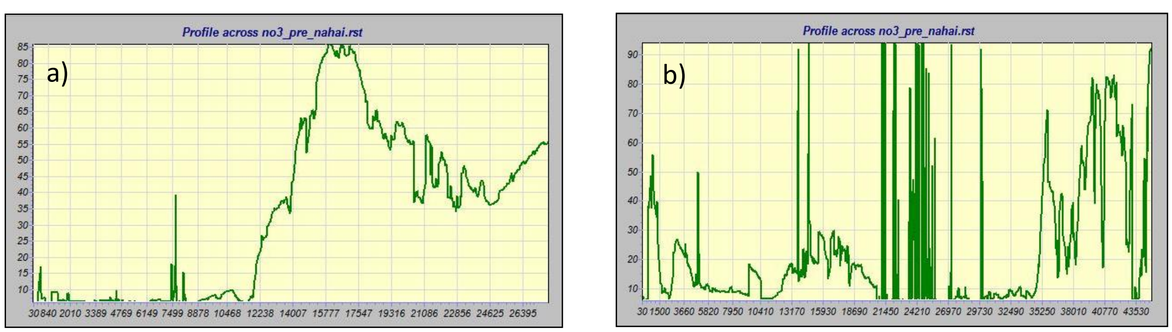

Figure 4. (a) North-South Profile and (b) West-East Profile of Nitrate Ion Prediction

Figure 3 shows that the amount of nitrate in the south and southeast of Tehran in the regions of 19-16-12-11-17 and also in the eastern end of Tehran located in region 4 is higher than other regions and the study of the north-south profile (Figure 4). It indicates an increase in ion concentration from north to south and the west-east profile indicates an increase in ion concentration in the central part of the city. The results obtained from the network sensitivity analysis show the greatest effect of the water table level and population density parameter on increasing the nitrate concentration. This means that southern regions with higher water levels and population densities have shown higher levels of nitrate. The north-south profile indicates an increase in ion concentration from north to south and the west-east profile indicates an increase in ion concentration in the central part of the city. The results obtained from the network sensitivity analysis show the greatest effect of the water table level and population density on increasing the nitrate concentration. This means that southern regions with higher water table levels and population densities have shown higher levels of nitrate.

3.2 Kriging interpolation method

By examining and comparing the mean standard error in different kriging methods and different Semivariogram models, the best level of prediction for the available data was obtained by choosing Ordinary kriging method and Spherical model. According to the mentioned method and model, the distribution of nitrate in the groundwater level is shown in Figure 5. Since the kriging method is based on interpolation using neighborhood points, the predicted maps are based on the values of the adjacent piezometric wells. Therefore, the predicted values of the nitrate parameter are affected by their measurements. Therefore, interpolation means the conversion of point data into area data. The accuracy of the selected models was assessed by trial and error through cross validation and RMSE comparison.

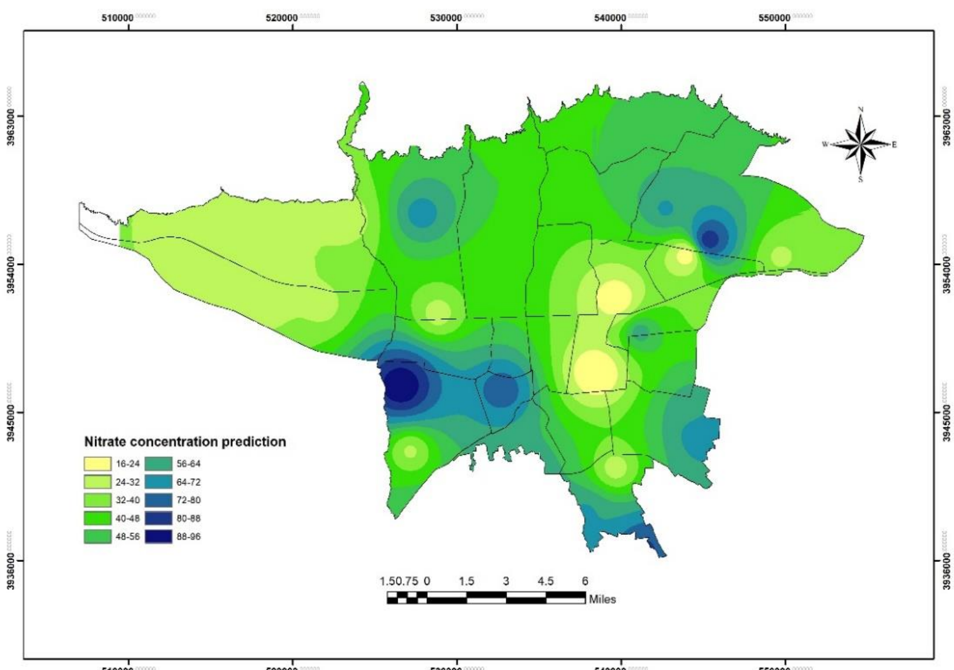

Figure 5. Nitrate ion prediction map by Kriging method

3.3 Comparison of Models

3.3.1. Comparison using Statistical Method of T-Student Test

After performing the above steps to compare the two prediction methods with each other, t-student test at 95% confidence level was used. The results of the two predictions have a non-significant relationship with each other. The results are as shown in Table 5:

Table 5. Comparison of Two Methods with T Test

Parameter name	Type of relationship	Comparison of two methods of t-student test
Nitrate	insignificant	0.918

3.3.2. Comparison using VALIDATE statistical method in GIS environment

VALIDATE is a statistical method by which the degree of agreement between two maps with IMAGE architecture and integer or byte format is examined. After performing the test, if there is more disagreement, then it can be concluded that the two models under study are different in prediction. Otherwise, if the two models have more agreement than disagreement, then the predicted results are similar. The desired results in the present research are given in Table 6.

Table 6. Comparison of two methods using VALIDATE test

Parameter name	Type of relationship	Comparison of two validate methods
Nitrate	Disagreement	0.0105

4. Discussion

The purpose of this study was to investigate the possible relationship between the types of land uses and the amount of groundwater nitrate using artificial neural network in the aquifer of Tehran. The type of neural network used in this study was a multilayer perceptron (MLP) network. In general, several layers with different numbers of neurons were used to evaluate the function of the perceptron network. After training the network, the RMSE of the training network was calculated and based on it, the most appropriate optimal model was selected. Among all the activation functions, the application of the hyperbolic tangent threshold function showed better performance. The network with 1000 training cycles, the hyperbolic tangent threshold function with post-diffusion algorithm s produced the lowest training error compared to other network architectures. This architecture predicted changes in groundwater nitrate with acceptable coefficients of determination. Application of multilayer perceptron neural network provided better results than the kriging interpolation. The results show the potential of the neural network as a tool to predict changes in groundwater nitrate. In several stages, data preparation and necessary corrections were made on the inputs and outputs. These modifications included selection of the appropriate resolution for modeling and the most important factors affecting groundwater nitrate concentration. Several rounds of trial and error showed 30 meters as the best resolution for the maps that were going to be used in the neural network model.

The results of sensitivity analysis showed that the effect of independent variables on the dependent variable is different. In general, the independent variables including geology, water table level, population density and digital elevation model had the highest effect on ground water nitrate concentration while precipitation and distance from river variables had moderate effect and distance from vegetation, slope and distance from main streets showed the least effect on nitrate. Elimination of high-effect variables had a significant reduction in the model accuracy. Moderate-effect variables and low-effect variables had a decreasing effect on model selection at the time of removal. We found that water table, geology, population density and elevation had great effect on groundwater nitrate in the study area.

To examine the similarity of the two models, their predictions were compared using two statistical tests. The results of t-student test showed that a significant difference between the estimated data of the two models. Also, VALIDATE module in Idrisi was used to compare the similarity of the prediction maps of the two models and the results showed that disagreement is higher than agreement between the two maps. That is, the two models are significantly different in terms of forecasting. In the present neural network, significant correlations were observed between the observed and predicted parameters, which are mentioned in above tables indicating that the network has predicted the parameter with high accuracy. The RMSE in neural network predictions was much smaller than that of the kriging method. The same issue was confirmed in the study of Tavassoli et al. (2022).

According to the results of the study of Tavassoli et al. (2022), it was determined that the performance of the Kriging method in spatial prediction is stronger than that of the neural network, but it is still a significant method. Therefore, it can be concluded that the neural network model is more accurate in prediction, which has been confirmed by Secci et al. (2015) and Bowers et al. (2022).The results of their study showed that the artificial artificial network estimates the depth of the layer better than the kriging method. However, the greater advantage of kriging over artificial neural network methods is that it can simulate spatial diversity and show it quickly on a map. The main reason that the neural network model is more accurate than the kriging method is that the network is trained based on the value of the parameter and responds in the end on the same basis. In addition, the ability to influence the factors that cause a phenomenon in predicting it in the neural network model, instead of using the phenomenon itself to predict, makes understanding the relationships between factors, the effect of factors weight on the values of the phenomenon, causation and plotting the spatial distribution from a zonal shape to a point shape (Secci et al., 2015). As a result, it increases the ability to analyze and predict compared to the kriging method. This study has shown that artificial neural networks superior to the Kriging model in estimating the groundwater quality parameter prediction. On the other hand, according to Şişman & Kizilöz (2020), the results of the kriging model are much better for estimation than the artificial neural network models. Tavassoli et al. (2022) also concluded that neural network performance in spatial prediction is weaker than the kriging method, but can still be a good competitor to kriging. Sen et al. (2008) compared the accuracy of artificial neural networks and kriging. Artificial neural networks provide sufficient accuracy for spatial interpolation, but Kriging interpolation predictions are more accurate.

In interpreting these results, it can be said that in artificial neural network models, evaluation through predictions is difficult. In these models, it is not possible to directly obtain information about why and how the results of the model. On the other hand, the development of innovative models that allow expert evaluation and interpretation is possible using the new kriging technique. In addition to the capabilities of the artificial neural network model versus the kriging interpolation model, there are limitations, which are the limitations of the neural network method in retraining (updating) to include new changes and re-predict with high accuracy. This is one of the main limitations of these methods. Also, this method has more error when using extrapolation because the data is in the range outside the trained data. This doubles the need to update data and models. Mijwel (2018) also stated the limitations of using an artificial neural network.

According to their study, artificial neural networks in accordance with their architecture need processors with parallel processing power. Unexplained network behavior is the most important problem of artificial neural network. When an artificial neural network offers a solution, it does not specify why, which is consistent with the results of the Şişman & Kizilöz (2020) study. This reduces trust in the network. There are no specific rules for determining the architecture of artificial neural networks. Proper network architecture is achieved through trial and error and experience.

5. Conclusion

The present study was conducted to predict the possible relationship between the types of land uses and the amount of groundwater nitrate in Tehran Metropolis using artificial neural network. In the process, the effects of land uses and the relationship between changes in the level of groundwater nitrate were also studied. The results of this study showed that the type of land uses in the study area affects the amount of nitrate in groundwater. Among these, we can cite the strong influence of the population density. Our results of network sensitivity analysis were similar to scientific findings regarding the factors influencing the formation of the nitrate in groundwater. Model outputs in the form of maps, tables and graphs allowed the study of the role of each variable and the extent of its impact on groundwater quality. This capability can lead to its use before the implementation of management policies by relevant organizations and water resources planners. On the other hand, one of the barriers to decision making is shortage of information. Predictive models help managers to make appropriate decisions by removing these barriers. On the other hand, creating multiple scenarios for the future or in unknown places is another capability of these kinds of modeling for decision makers and managers. According to the presented materials, performing various simulations and modeling of groundwater pollution provides an effective benchmark towards optimizing management, control, planning and decision-making leading to economic and environmental saving.

This research is limited by time, so to improve the research in this study there are several suggestions for future research such as (1) Using the network model output map as a tool to manage areas with low groundwater quality potential; (2) Implementing Tehran's urban sewage system in the medium term to prevent domestic wastewater from entering infiltration wells, which has led to an increase in groundwater levels in the southern region; (3) Managing variables that have a high impact on groundwater quality and controlling their intensity in areas of high concentration to prevent problems arising from an increase in these parameters, especially in the southern areas of the city; and (4) Reducing population density in areas where this factor is influential.

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