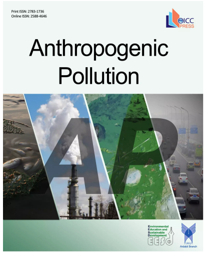

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Evaluation of temporal and spatial changes of irrigation water quality classes in Qazvin Plain, Iran, using machine learning models

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Original Research

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Abstract:

The present study aimed to determine the quality and quantity of groundwater resources for agricultural purposes in the Qazvin Plain (northwest of Iran) using the spatial and temporal distribution maps of agricultural water quality classes prepared by machine learning models during three study periods of spring 2012, 2016, and 2020. Modeling was performed based on geological maps, annual precipitation maps and 12 hydrogeochemical parameters measured for 63 piezometric wells. Appropriate hydrochemical parameters were selected for each statistical period to model agricultural water quality using the machine learning models of Random Forest (RF), Boosted Regression Tree (BRT) and Multinomial Logistic Regression (MnLR). The results introduced the best models to be RF in 2012 (kappa coefficient ($\kappa = 0.54$, overall accuracy (OA)= 69%) and MnLR in 2016 and 2020 ($\kappa = 0.83$ and 0.75; OA = 88 and 84%), respectively. The percentage of area for C4-S3 class (very high salinity with high sodium) increased from 5% in 2011 to 23.9% in 2019. Giving the increased precipitation in 2019, the agricultural water quality class in the southern region changed from C4-S3 in 2015 to C4-S2 (very high salinity with medium sodium) in 2019. Additionally, the simulated maps showed an elevation in the percentage of C4-S3 class area from 2012 to 2020 in the central part of the region where agricultural lands are concentrated. Our findings revealed the trend of adverse changes in water quality at different regions of Qazvin Plain during the years of study, highlighting the need to make purposeful management decisions. And The study utilized both advanced machine learning algorithms and traditional classification methods, including the Wilcox diagram, to assess agricultural water quality based on twelve physicochemical parameters. And The 12 parameters used in the study were selected based on data availability and relevance to agricultural water quality standards. Due to inconsistent data across years, variables such as nitrate and organic matter were excluded.

Keywords: Spatial distribution; Water resource quality; Machine learning models; Qazvin Plain

1. Introduction

The scarcity of surface water resources in arid and semi-arid regions today has made underground water one of the most important and valuable water sources in such areas (Mohammadi et al., 2023). Hence, comprehensive exploration and proper exploitation of these water resources can significantly affect sustainable development and various agricultural and socio-economic activities in such regions (Eslaminezhad et al., 2022; Masoudi et al., 2023). Following the growth of the population and the subsequent increase in the demand for water in diverse sectors of agriculture, drinking and industry, the overexploitation of groundwater resources has caused a decrease in the quality and an increase in the pollution of these valuable resources, which can leave irreparable effects on the agriculture sector and especially on the health of society (Bui et al., 2020; Jalili, 2020). Accordingly, the management of groundwater resources worldwide has become a critical issue in recent decades.

Groundwater sources provide drinking water for 50% of the world's population (Jiang et al., 2022) and also constitute 43% of the total agricultural water (Li et al., 2002; Fataei and Shiralipoor, 2011). Groundwater resources are one of the basic needs of the agricultural sector, especially in arid and semi-arid areas where there is a shortage of surface water (Dehghan Rahimabadi et al., 2022; Valiallahi, 2022). Proper management and exploitation of groundwater resources requires quantitative and qualitative evaluation and monitoring of water resources in order to minimize damage to the environment and reservoirs of these waters via their optimal usage.

Considering the effects of climate change, such as increasing global warming, decreasing rainfall, and extreme climatic events, a unique approach is needed to study the effects of climate elements on groundwater level changes, which can help in better decision making. Recent years have seen the increasing use of machine learning and data-driven methods for groundwater modeling. Applying data-based methods, spatial databases and developing machine learning techniques based on non-linear interdependencies can help predict groundwater level change. New machine learning methods and mathematical model techniques have recently made a significant contribution to the prediction of groundwater level fluctuations; these methods have been found to help simplify and eliminate complexity in calculations. According to previous findings, machine learning methods could provide higher accuracy in the prediction process compared to mathematical models. However, some researchers recommended the integration of machine learning and mathematical models to predict groundwater level changes (Afrifa et al., 2022). Machine learning methods are capable of identifying hidden patterns in data and then applying those patterns to predict target variables or parameters (Masoudi et al., 2023).

Researchers have applied a variety of machine learning models for groundwater modeling, including artificial neural network, ANN (Adamowski and Chan, 2011; Nourani et al., 2015; Oliveira et al., 2023), fuzzy theory, FT (Zhang, 2015; Jeihouni et al., 2019), genetic programming, GP (Naghibi et al., 2017; Sepahvand et al., 2019) and support vector machine, SVM (Dehghani et al., 2022). In this regard, a study evaluated the potential of groundwater resources based on environmental factors in the Yasouj-Sisakht area, Iran, using Random Forest (RF) and Generalized Linear Model (GLM). In this research, 12 layers of environmental predictors were used as the most important factors influencing groundwater potential. The results of the relative importance of factors affecting the potential of groundwater resources in these methods showed that rainfall, altitude and distance to fault were the most sensitive factors. Additionally, the accuracy of the models was evaluated by the receiver operating characteristic (ROC) curve; accordingly, the area under curve (AUC) was calculated to be 92% and 65% for the RF and GLM models, respectively, indicating the higher accuracy of the RF model in mapping groundwater potential compared to the GLM (Avand et al., 2019). In a study,

Accordingly, in different regions of the world, including the Qazvin plain, which is one of the most important agricultural regions of Iran, it is vital to identify the parameters affecting water quality. Due to the lack of surface water resources in the Qazvin Plain, more attention needs to be paid to the purposeful exploitation and management of groundwater resources.

To the best of our knowledge, since no study has been done on water resource management, as well as temporal and spatial distribution maps of water quality parameters using machine learning models in the Qazvin Plain, extensive and comprehensive research in the field of water resources management and groundwater quality modeling of the Qazvin plain using machine learning approaches can be a suitable guide for planning and adopting management strategies compatible with groundwater. Correspondingly, the purpose of this research was to determine the most important parameters affecting groundwater quality considering the effect of drought index (standardized precipitation index, SPI) and mean annual precipitation (MAP), and to investigate the potential of RF, boosted regression tree (BRT) and multinomial logistic regression (MnLR) models in distribution and prediction of groundwater quality based on USSL diagram and finally to map the groundwater quality classes for agricultural use in Qazvin Plain.

2. Materials and models

2.1 Study area

Qazvin plain is located in the middle of $35°18'$ to $36°30'$ northern latitude and $49°11'$ to $50°40'$ eastern longitude. The area of the studied plain is 952,623 hectares and its altitude varies from 952 to 2911 meters, so that the central and eastern parts of the plain have a lower altitude than the northern, western and southern regions. Figure 1 illustrates the geographic location of the studied area and the studied piezometric wells.

The land use map of the region reveals that agricultural lands (29.47% of the region's area), behind barren lands (41.54% of the region's area), occupy the largest share in the Qazvin plain, thus indicating the position of agricultural activities in the region (Fig. 2). Discontinuous sediments, including new terraces and alluviums, cover the largest area (574,468 hectares) in the plain. In these Quaternary formations, water infiltration rate and permeability are very high and they form the bed of very large aquifers, subsequently developing groundwater sources in these formations (Fig. 3).

In terms of climatic factors, the lowest average annual temperature in the Qazvin Plain is 2 °C, which is observed in the northern and northeastern highlands of the region. In the central and flatten parts of the plain and the inner parts of the province, the average annual temperature reaches 14.5 °C (Abdullahi Dehki, 2019). According to the MAP (256.6 mm) and average annual temperature (13.5 °C) in Qazvin plain, this plain has an aridity index of 10.92, which has a semi-arid climate based on De Martonne climatic classification. The rivers flowing in the Qazvin plain eventually lead to Namak Lake. Abhar, Chay Khar Rud, Haji Arab rivers join Kordan River and form Shur River, which finally drains into Namak Lake (Abdullahi Dehki, 2019).

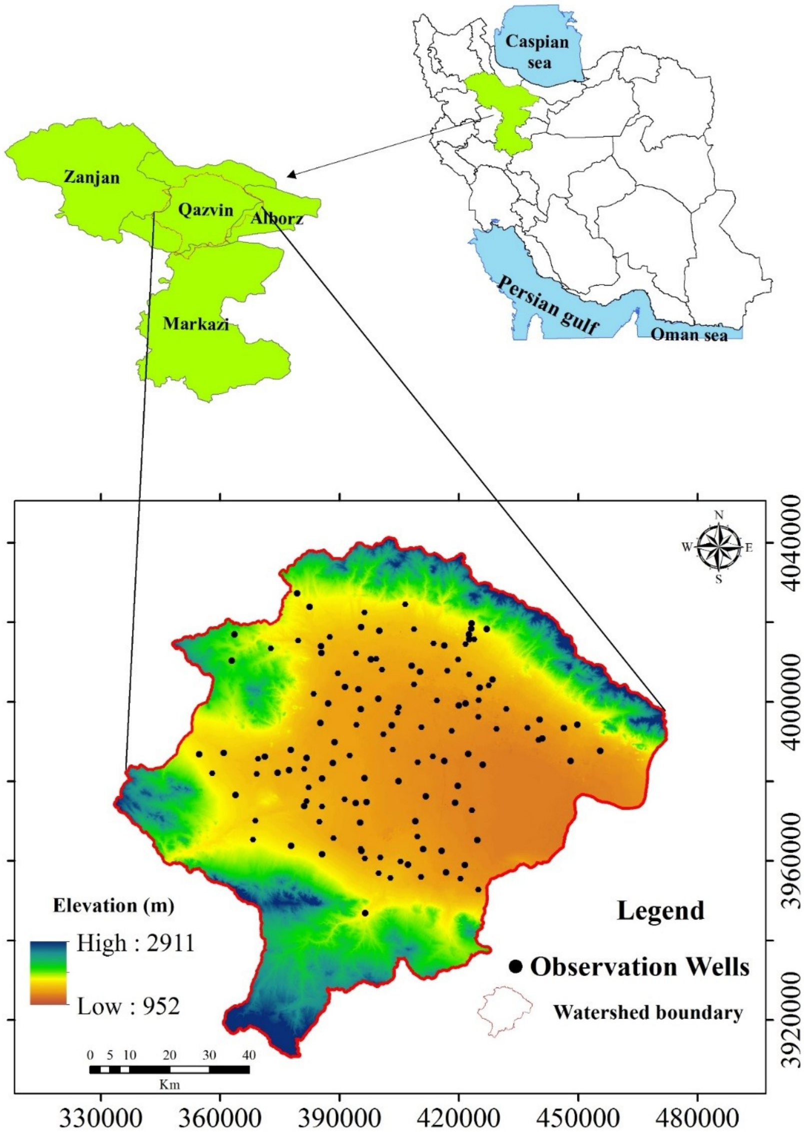

Figure 1. Location of Qazvin plain relative to the existing provinces in Iran and spatial distribution of the studied piezo-metric wells.

2.2 Methodology

In the current research, temporal and spatial changes in the quality of agricultural water in Qazvin Plain were generally designed and investigated in seven basic steps as follows:

1. Collecting and normalizing data related to water quality parameters for the spring of 2012, 2016 and 2020
2. Determining the most suitable chemical parameters of water quality using principal component analysis (PCA)
3. Determining the agricultural water quality classes of each well according to the USSL diagram
4. Spatial modeling of agricultural water quality into two groups of training (80%) and testing (20%)
5. Modeling the agricultural water quality index using RF, MnLR and BRT machine learning models in R software
6. Determining the most appropriate water quality parameters in each period based on their relative importance
7. Mapping the spatial and temporal prediction of agricultural water quality during the studied years and mapping the SPI in Arc GIS software

In this research, groundwater quality data was provided from the IRAN Water Resources Management Company. According to the available statistics, 12 hydrogeochemical parameters, including potassium (K^+), sodium (Na^+), magnesium (Mg^{2+}) and calcium (Ca^{2+}) as major cations, sulfate (SO_4^{2-}), chloride (Cl^-) and bicarbonate (HCO^{3-}) as major anions, pH, total hardness (TH), electrical conductivity (EC), total dissolved solids (TDS), and sodium adsorption ratio (SAR), measured for 63 sampling wells were considered as inputs to determine the groundwater quality in the Qazvin plain during the years under study. Normalization, if needed, was done for all the parameters related to 2012 by logarithmic transformation method and to

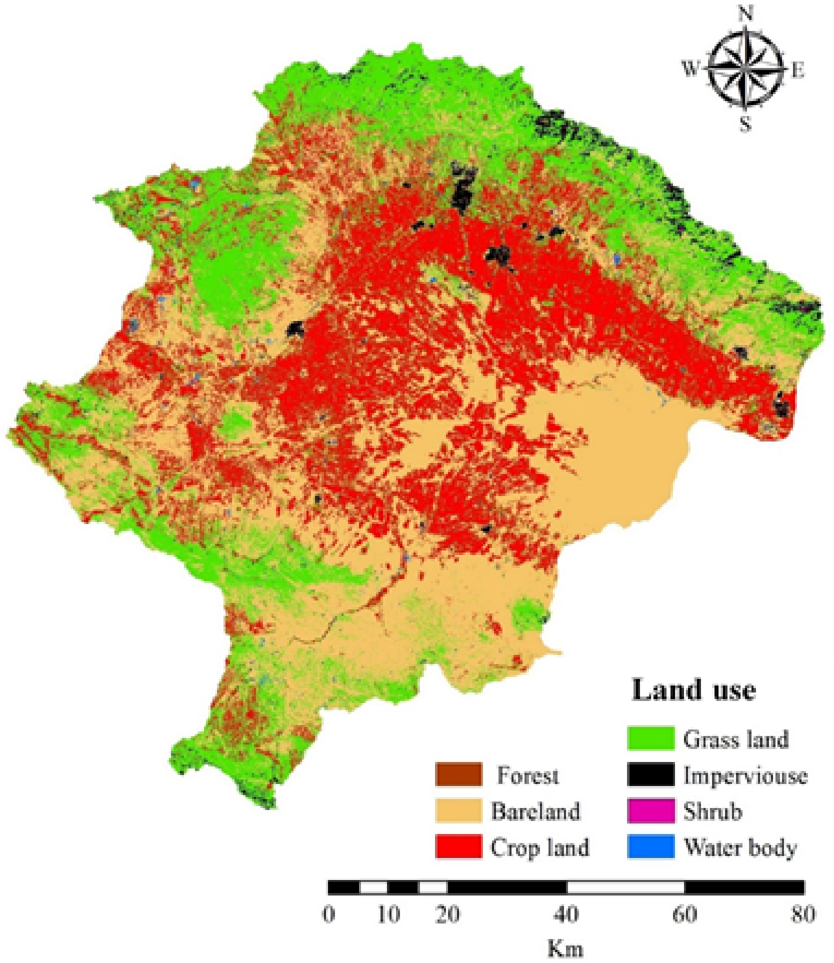

Figure 2. Land use map of Qazvin Plain, Iran.

2016 and 2020 by SPSS version 21 software and integrated method (ranking of cases and computation of variables).

2.3 Selection of hydrochemical and environmental factors

In this part of the research, two methods of PCA (Pallant, 2020) and expert opinion were used to select the most suitable dataset among the tested quality parameters and environmental variables to reduce the interference between parameters and determine the most effective ones. Therefore, among the 12 measured hydrochemical factors for each statistical period, the most appropriate ones were selected based on the PCA approach. Simultaneously with the hydro-chemical characteristics, the geological maps of the studied area as a representative of the parent material of the main producers of the area and the MAP as an effective climatic index in drought were prepared as input data for modeling. In addition to the mentioned factors, the maps of SPI and water elevation contour were also drawn in 135 wells to investigate and interpret the changes in groundwater quality and influencing factors as well as possible.

2.4 Determination of agricultural water quality class

The water quality class with a discrete nature was determined to identify agricultural use based on the USSL diagram (Table 1).

Table 1 Classification of agricultural water quality for agricultural purposes based on the USSL diagram (US Salinity Laboratory Staff 1954).

2.5 Spatial modeling of groundwater quality

Data mining is the analysis of a large set of data in order to reveal hidden and significant patterns and rules within the data (Gorunescu, 2011). In this research, three RF, BRT and MnLR algorithms were used to predict the spatial distribution of agricultural water quality; the structure of these three algorithms is briefly discussed below:

2.5.1 Random Forest model

One of the algorithms used in this research was the RF model presented by Breiman (2001). This model is developed from the Classification and Regression Tree (CART) model that separates the data iteratively to obtain the relationship between the target variable and the independent variables, and perform estimation. Unlike other tree-based algorithms that draw a limited number of trees, hundreds or thousands of classification trees are generated in the RF method (Breiman and Cutler, 2005). It is a group learning model and works for classification by building a large number of trees (Breiman, 2001).

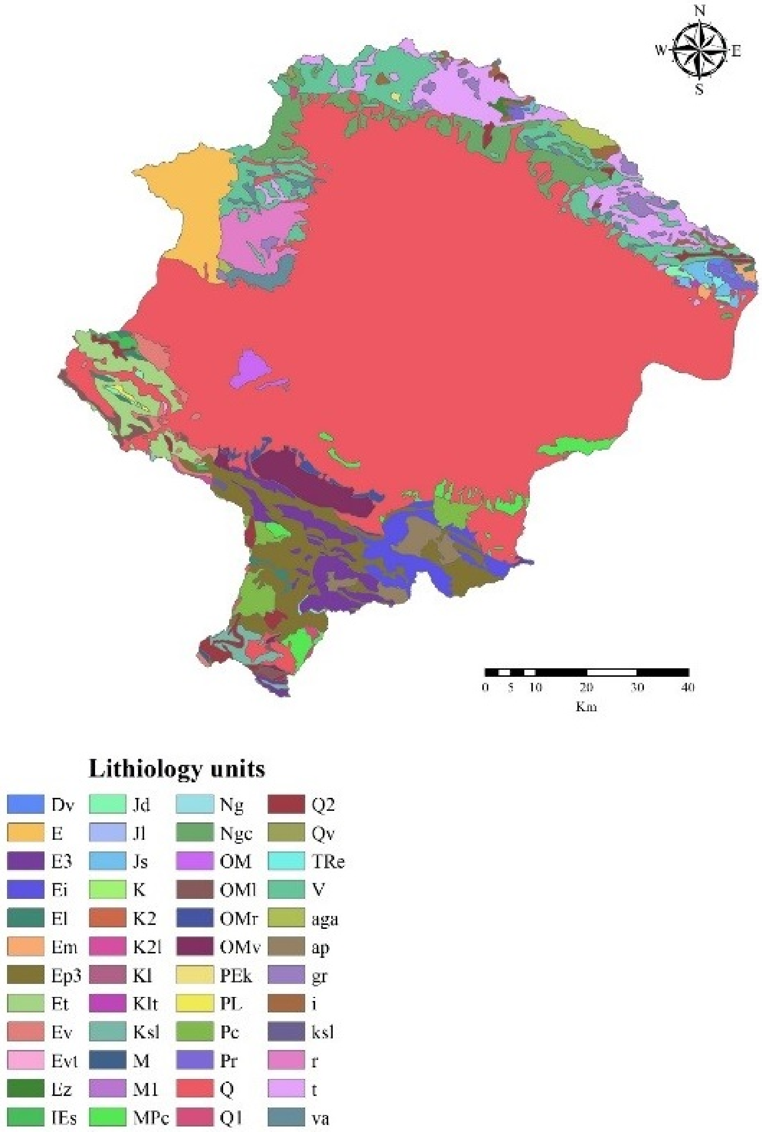

Figure 3. Geological map of Qazvin Plain, Iran.

2.5.2 Boosted Regression Tree model

This algorithm improves the fit of a model by adapting several other models and integrating them to make model predictions. BRT is one of the subsets of decision tree, which has been greatly developed in the last two decades. The BRT model uses two groups of regression tree and decision tree algorithms, on the one hand, and the combination of a set of models along with their boosting, on the other hand. Boosting is a machine learning technique that integrates the results of multiple model comparison (Jafari et al., 2014; Elith et al., 2008).

2.5.3 Multinomial Logistic Regression

Logistic models are a special type of generalized linear models (GLMs), which can be implemented in two ways: 1- Binomial logistic model and 2- Multinomial logistic model. In the binomial logistic model, the dependent variable is in the form of presence or absence (zero and one); for example, the presence or absence of a characteristic soil horizon,

Table 1. Classification of agricultural water quality for agricultural purposes based on the USSL diagram (US Salinity Laboratory Staff 1954).

Classes	Water quality for agriculture
C1S1	Sweet, completely effective for agriculture
C2S1,C2S2,C1S2	Brackish, approximately perfect for agriculture
C1S3,C2S3,C3S1,C3S2,C3S3	Passion, usable for agriculture
C1S4,C2S4,C3S4,C4S4,C4S3,C4S2,C4S1	Very passion, harmful to agriculture

while Multinomial logistic model covers the dependent variable with several classes, such as different classes of soil in the same area.

2.6 Model validation test

In this study, the validation method or the test sample was used to evaluate the validity of the models used. To this end, 80% of the data of groundwater wells were used for measuring the accuracy of the model and 20% of the data were used for the validation of the model. The criteria of overall accuracy (OA) and Kappa coefficient (κ) were used to evaluate the accuracy of the classification, which are as follows (Byrt et al., 1993).

2.7 Overall accuracy

In Eq. (1), OA represents overall accuracy, N represents all classified pixels, and $\sum_{i=1}^{n} X_{ij}$ represents the total pixels of the main diameter of the error matrix (correctly classified pixels). OA cannot provide information about each of the classes separately.

$$\mathrm{OA} = \frac{\sum_{i=1}^{n} X_{ij}}{N} \tag{1}$$

2.8 Kappa coefficient

The kappa statistic is a powerful index that calculates the probability of presence or absence of classes correctly predicted by the model; Therefore, it is always slightly less than the map purity. The range of Kappa statistic changes is between zero and one (Jafari et al., 2014). In Eq. (2), n stands for the number of rows in the matrix, X_{ij} for the number of observations in row i and column j (main diameter entries), X_{io} and X_{oi} for the sum of the margins in row r and column i respectively, N for the total number of observations.

$$\mathrm{Kappa} = N\sum_{i=1}^{n} X_{ij} - \frac{\sum_{i=1}^{n}(X_{io} - X_{oi})}{N^2} - \sum_{i=1}^{n}(X_{io} - X_{oi}) \tag{2}$$

3. Results and discussion

In addition to machine learning models, the Wilcox diagram was applied to classify irrigation water quality based on salinity hazard (EC) and sodium hazard (SAR). This traditional method enables a comparative assessment of water usability for agriculture. The water samples from different years (2012, 2016, 2020) were plotted on the Wilcox diagram to provide a standard reference framework. Results obtained from Wilcox classification were then compared with outputs from the applied machine learning models.

3.1 Statistical description of agricultural water quality factors

After normalizing the agricultural water quality data, the most suitable ones were selected by PCA method for all three years 2016, 2012 and 2020 separately, as shown in Tables 2, 3 and 4. Based on the results of the PCA method for the statistical year 2012, EC, pH and HCO^{3-} had eigenvalues greater than one. In this regard, TDS and HCO^{3-} for 2016 and EC, pH, K and HCO^{3-} for 2020 had the highest weight, respectively.
The statistical summary of each of the selected factors of agricultural water quality by the years under study is presented in Table 5. According to

Table 5, the mean concentration of HCO^{3-} was 3.79 milliequivalents per liter (mEq/L), with the minimum and

Table 2. Matrix of components related to agricultural water quality factors in spring 2012 in Qazvin Plain, Iran.

	Quality factors	Ca^{2+}	Mg^{2+}	Na^{+}	K^{+}	EC	SAR	TH	TDS	pH	HCO^{3-}	Cl	So_4^{+}
Principal components	PC1	0.85	0.93	0.94	0.87	0.99	0.81	0.95	0.99	-0.50	-0.008	0.95	0.89
	PC2	-0.42	-0.06	0.29	0.17	0.06	0.50	-0.24	0.07	0.60	0.353	0.20	-0.24
	PC3	-0.08	0.052	-0.01	0.001	-0.035	-0.039	-0.008	-0.034	-0.51	0.91	-0.09	-0.02

Table 3. Matrix of components related to agricultural water quality factors in spring 2016 in Qazvin Plain, Iran.

	Quality factors	Ca^{2+}	Mg^{2+}	Na^{+}	K^{+}	EC	SAR	TH	TDS	pH	HCO^{3-}	Cl	So_4^{+}
Principal components	PC1	0.828	0.893	-0.94	0.70	0.99	0.77	0.93	0.99	-0.518	-0.210	-0.956	0.890
	PC2	0.238	0.150	-0.163	0.089	-0.017	-0.322	0.211	0.019	-0.396	0.772	-0.199	0.132

Table 4. Matrix of components related to agricultural water quality factors in spring 2020 in Qazvin Plain, Iran.

	Quality factors	Ca^{2+}	Mg^{2+}	Na^{+}	K^{+}	EC	SAR	TH	TDS	pH	HCO^{3-}	Cl	So_4^{+}
Principal components	PC1	0.843	0.874	0.917	0.26	0.993	0.645	0.918	0.99	-0.265	-0.054	0.925	0.765
	PC2	-0.256	-0.207	0.306	-0.621	0.083	0.557	-0.252	0.08	0.673	-0.178	0.08	0.102
	PC3	-0.251	-0.148	0.168	0.246	0.018	0.409	-0.223	0.00	-0.201	0.899	-0.262	0.358

Table 5. Statistical summary of selected parameters for modeling agricultural water quality in Qazvin Plain, Iran, during three study periods of spring 2012, 2016, and 2020.

Study periods	Parameters	Unit	Minimum	Maximum	Mean	standard deviation	Coefficient of variation (CV%)	Skewness	Kurtosis	Transformation method
2012	HCO^{3-}	mEq/L	1.69	5.52	3.79	0.87	22	-0.44	-0.30	-
	pH	-	7.10	8.20	7.67	0.25	3.32	0.14	-0.52	-
	EC	mS/cm	481	6523	1842	129	70	1.42	2.31	Logarithmic
2016	HCO^{3-}	mEq/L	0.80	9.20	4.22	1.55	36.8	0.75	1.72	-
	TDS		216	4317	1036	794	76.6	2.27	6.90	Integrated
2020	HCO^{3-}		1.02	7.18	4.06	1.28	31.7	0.321	0.132	-
	pH	-	7.33	8.71	7.97	0.28	3.6	0.075	-0.153	-
	K		0.02	0.82	0.09	0.11	116	4.98	31.8	Integrated
	EC	mS/cm	3.72	6689	1731	1130	65.3	1.40	4.60	Integrated

maximum concentrations of 1.69 and 5.52 mEq/L in the spring 2012. The minimum, mean and maximum pH values were 7.10, 7.67, and 8.20, respectively; the maximum values of this factor in the region seem to be in the alkaline class, which can make the soil of the region face the risk of sodification. The mean EC value was 1842 millisiemens/meter (mS/m), with minimum and maximum values of 481 and 6523 mS/m.

The mean concentration of HCO^{3-} and TDS in 2016 was 4.22 mEq/L and 1036, respectively, which were considered as selected quality parameters. For 2020, HCO^{3-}, pH, K and EC were selected as four qualitative parameters for data mining. EC with a minimum value of 3.72 mS/m and a maximum value of 6689 mS/m showed a wide range of changes in this year. In addition, the maximum value of pH (8.71) was in the alkaline class.

3.2 Spatial distribution of agricultural water quality factors

Table 6 shows the semivariogram fitted for each selected qualitative parameter.

The results of fitting the experimental semivariogram on the parameters affecting the agricultural water quality in the region showed that the exponential and spherical models were the most appropriate fitting in most of them, respectively. In terms of spatial dependence class, all of them were in the medium class, except for the EC factor in 2012 and 2020, TDS in 2016, and pH in 2020, which were in the strong class (Cambardella et al., 1994). Similar results were observed in the geostatistical analysis of agricultural water quality factors in Fars province, Iran (Masoudi et al., 2023). The strong and medium spatial dependence of agricultural water quality factors indicates that the use of geostatistical methods can be useful in the spatial analysis of the studied characteristics (Mousavi et al., 2017).

And One of the important but often overlooked factors affecting groundwater quality is the geological structure and lithology of the aquifer. The presence of evaporite and carbonate rocks, which are rich in soluble salts, plays a significant role in elevating the salinity and electrical conductivity of groundwater. Studies such as Ebadati (2016) in the Qazvin Plain have shown that geological formations, particularly sedimentary layers containing gypsum and halite, significantly impact groundwater chemistry. Therefore, incorporating lithological information is essential for a more comprehensive understanding of spatial variations in wa-

Table 6. Agricultural water quality parameters and the most appropriate model fitted on the semivariogram of water quality parameters in Qazvin Plain, Iran, during three study periods of spring 2012, 2016, and 2020.

Study period	Water quality parameters	Semivariogram model	Block variance (C_0)	Threshold (C)	Impact range (meters)	Spatial dependence (C_0/C)
2012	HCO^{3-}	Spherical	0.02	0.04	17539	Medium
	pH	Exponential	0.0005	0.00096	109040	Medium
	EC	Spherical	0.1	0.50	58975	Strong
2016	HCO^{3-}	Exponential	0.43	0.95	8373	Medium
	TDS	Spherical	38649	600180	45321	Strong
2020	HCO^{3-}	Stable	0.13	0.45	42813	Medium
	pH	Exponential	0.0093	0.07	8781	Strong
	K	Gaussian	0.2	0.37	9210	Medium
	EC	Exponential	321330	1460700	52807	Strong

ter quality. Previous research has explored the geological influence on groundwater quality in the Qazvin region. **Ebadati2016<empty citation>** highlighted the relationship between lithological composition and salinity variations across the plain, emphasizing the importance of geological mapping in water quality management strategies.

The spatial distribution map of water quality parameters in all three periods was drawn using ordinary kriging method (Fig. 4, 5 and 6). This method is the best unbiased predictor in random sampling in unsampled areas. Another advantage of this method is to reduce the impact of outlier points (Triantafilis et al., 2001).

In 2012, the highest value of EC was in the central part towards the south and east, and the lowest value was observed in the northern and western parts of the region. The highest pH value was reported in the north and northeast parts and the lowest value was obtained in the west and south parts. The highest concentration of HCO^{3-} was observed in the northern, central and western parts and the lowest level was found in the eastern parts, a little towards the south. The pH value in the northern to eastern parts of the study area indicated the alkalinity of the groundwater.

In 2016, the spatial distribution map was drawn for TDS and HCO^{3-}, where the highest TDS value was observed in the central part towards the east and south, and the highest concentration of HCO^{3-} was found in the northern, western and central parts, and the lowest concentration of HCO^{3-} was recorded in the eastern part.

In 2020, the highest concentration of potassium was observed in the central parts towards the south and parts of the west, the highest EC value in the central part towards the east, and the highest concentration of HCO^{3-} in the northern and western parts. The pH value in the northeastern and eastern parts towards the center of the studied area indicated the alkalinity of the groundwater.

3.3 Maps of mean annual precipitation and standardized precipitation index

In order to investigate the effect of climatic factors in this study, SPI (Fig. 7) and MAP (Fig. 8) maps were prepared for all three periods of 2012, 2016 and 2020, using the inverse distance weighting (IDW) interpolation method.

The results of SPI maps (Fig. 7) showed that, in general, the amount of drought in the region improved slightly from 2012 to 2020, and the lowest amount of drought in 2012 was observed in parts of the northern regions that include high areas. In 2016, the lowest SPI values were observed in parts of the northern and eastern regions. In 2020, the lowest SPI values were found in the southern areas and a small part of the north, which were close to the highlands of the study area.

The MAP maps in 2012, 2016 and 2020 highlighted that the average rainfall had generally increased in the region. The highest amount of precipitation in 2012 and 2016 was related to the northern and northeastern regions, and the highest amount of precipitation in 2020 was related to the northern and southern regions, which have higher altitudes in the mountainous regions.

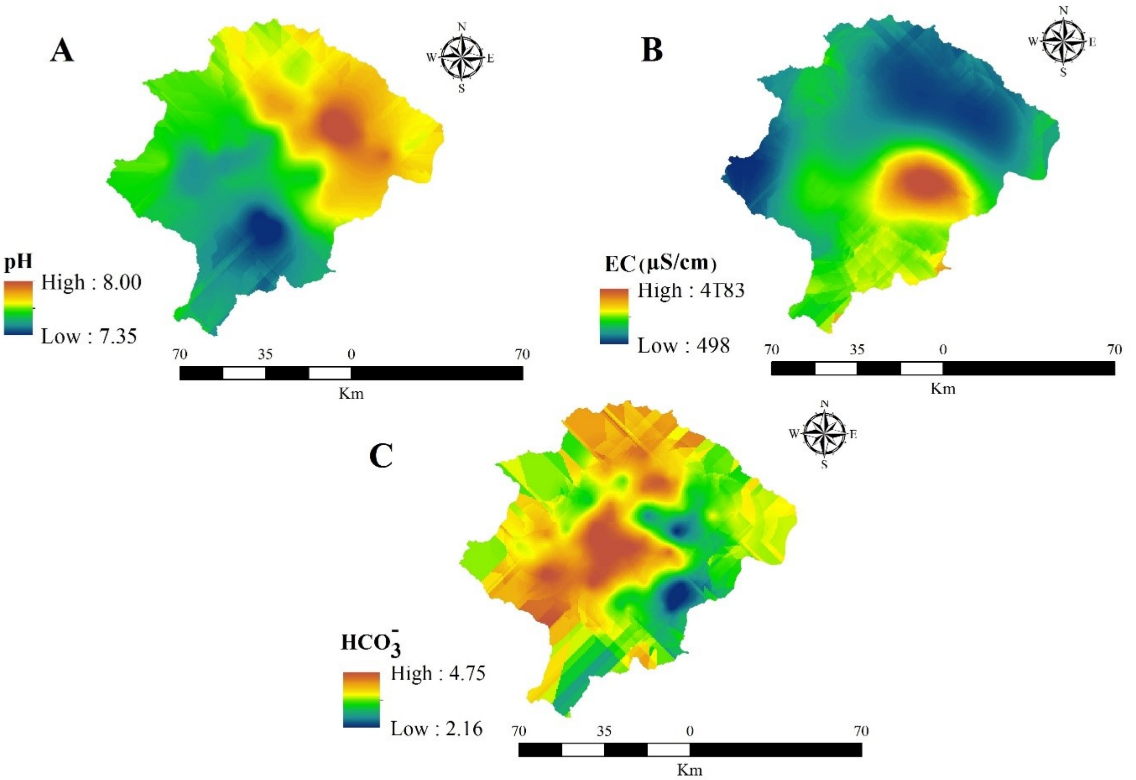

Figure 4. Distribution of selected quality parameters in 2012 based on the best semivariogram for each parameter in Qazvin Plain, Iran.

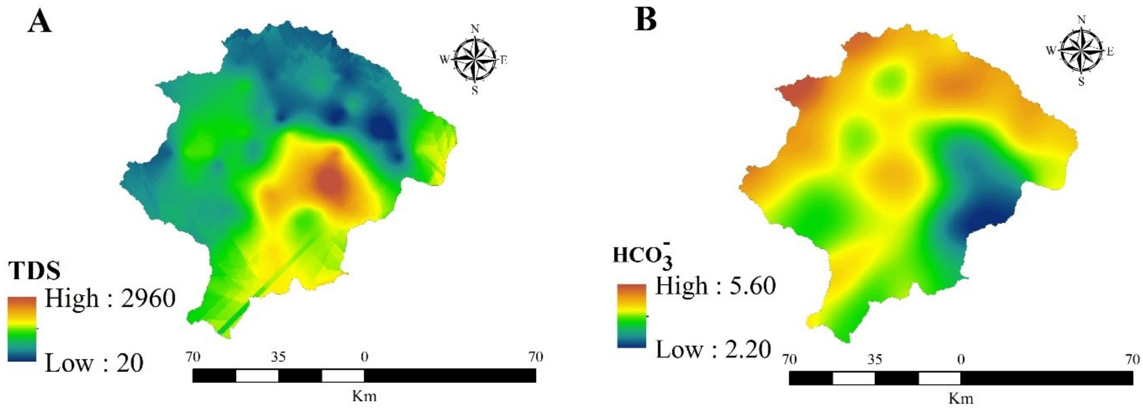

Figure 5. Distribution of selected quality parameters in 2016 based on the best semivariogram for each parameter in Qazvin Plain, Iran.

3.4 Evaluating the efficiency of machine learning models

Spatial modeling of agricultural water quality was done based on three machine learning models, RF, BRT and MnLR, and the results of comparing the efficiency of the used models based on the Kappa coefficient and OA indicators are presented in Table 7.

Comparing the efficiency of the models showed that the RF model provided the highest accuracy in spring 2012 ($\kappa = 0.54$, OA = 69%). In this regard, Jafari et al. (2021) used the RF model to predict the agricultural water quality class of Zayanderud River in Iran, the results of which were $\kappa = 0.88$ and OA = 96%. Another study compared the effectiveness of RF, BRT and MnLR data mining models in spatial prediction of groundwater resource quality. The results of all three methods showed acceptable accuracy for prediction during both study periods, but the results revealed that the RF model was more accurate than the other two regression models in predicting the agricultural water quality classes and spatial distribution of water quality parameters. These results indicated that the tree-based algorithm created between the target variable and hydrochemical parameters for the modeling process had increased the accuracy of the RF model compared to the BRT and MnLR models

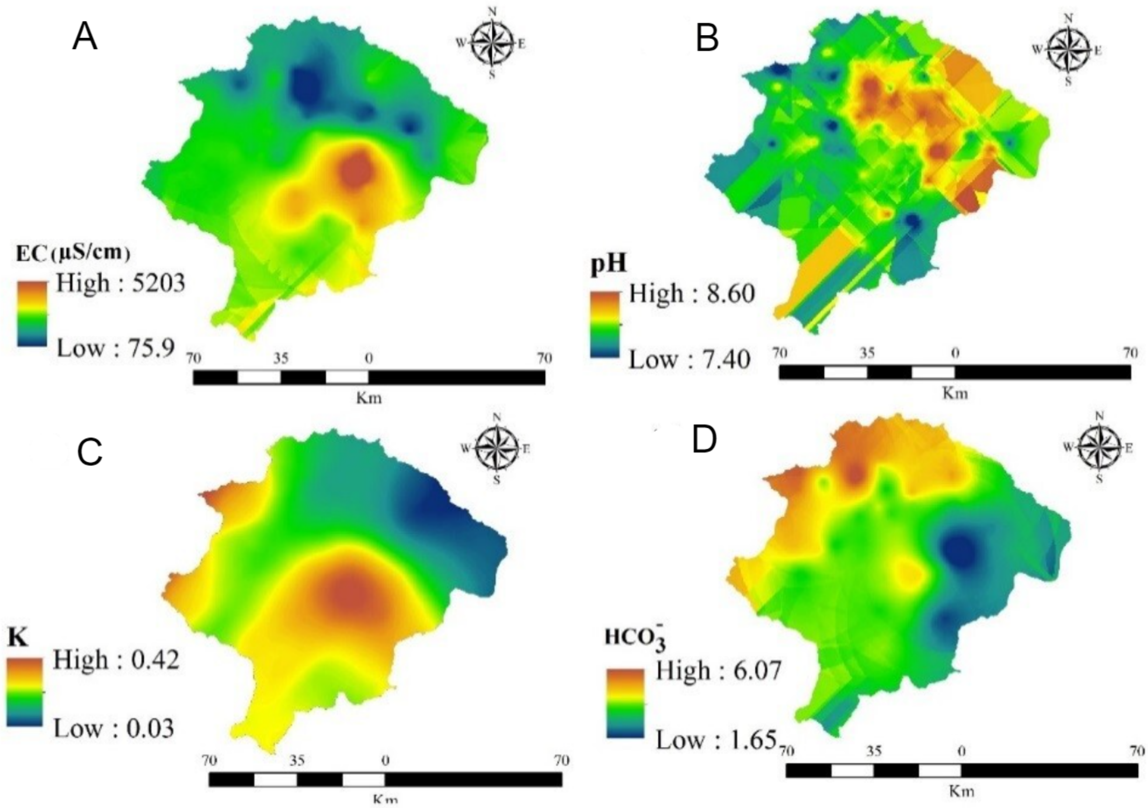

Figure 6. Distribution of selected quality parameters in 2020 based on the best semivariogram for each parameter in Qazvin Plain, Iran.

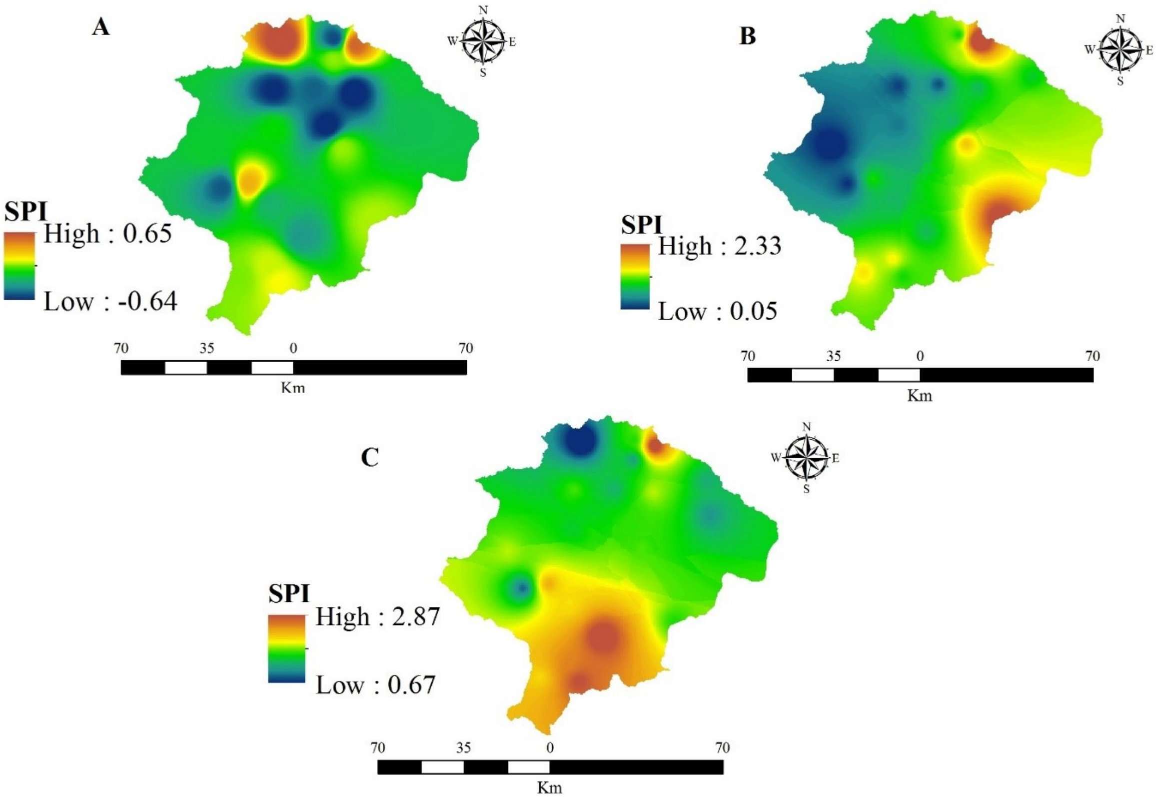

Figure 7. Spatial distribution of standardized precipitation index; (A) spring 2012, (B) spring 2016 and (C) spring 2020, in Qazvin Plain, Iran.

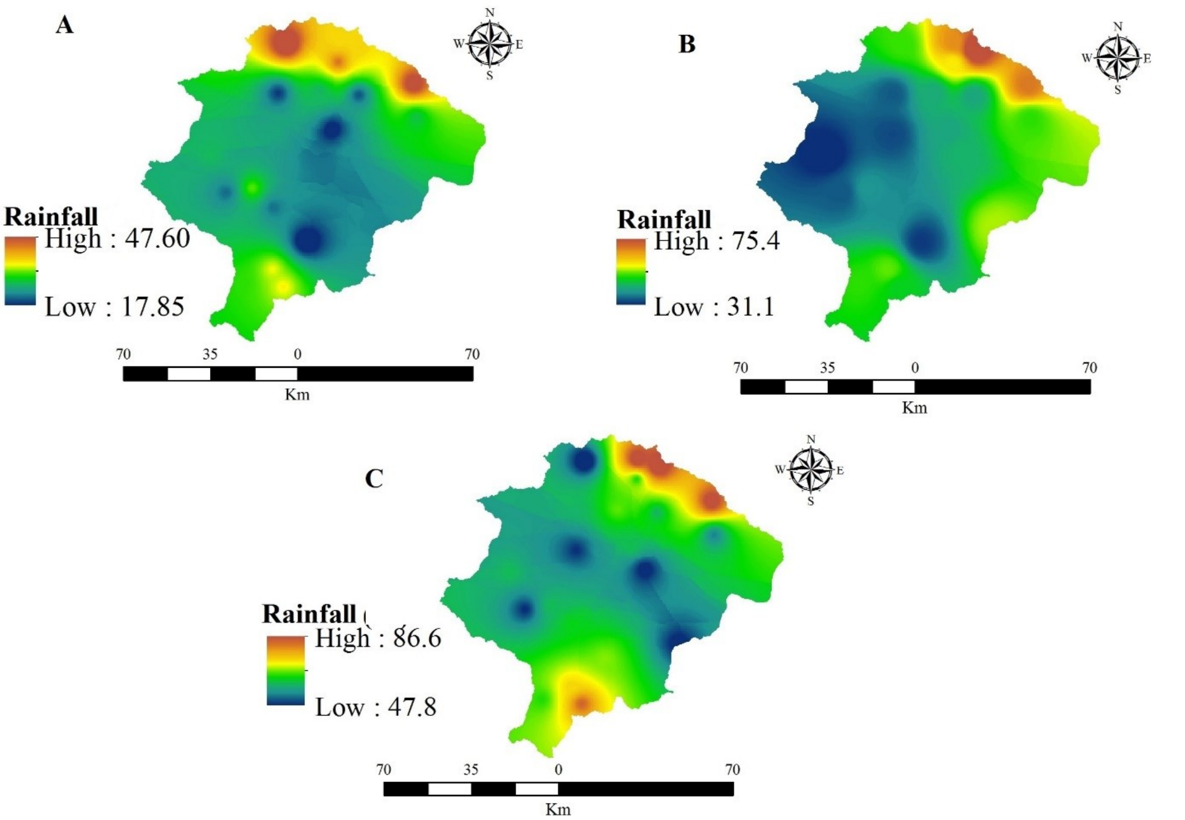

Figure 8. Spatial distribution of mean annual precipitation (MAP); (A) spring 2012, (B) spring 2016 and (C) spring 2020, in Qazvin Plain, Iran.

Table 7. Validation of the efficiency of machine learning models.

Study periods	Machine learning models	Validation	
		Overall accuracy	Kappa coefficient
Spring 2012	Random Forest	69	0.54
	Boosted Regression Tree	54	0.40
	Multinomial Logistic Regression	48	0.25
Spring 2016	Random Forest	81	0.71
	Boosted Regression Tree	72	0.52
	Multinomial Logistic Regression	88	0.83
Spring 2020	Random Forest	69	0.57
	Boosted Regression Tree	74	0.60
	Multinomial Logistic Regression	84	0.75

(Masoudi et al., 2023). In our study, the MnLR model in spring 2016 and 2020 with $\kappa = 0.83$, 0.75 and OA = 88, 84%, respectively, provided better performance than the RF and BRT models in predicting agricultural water quality classes. Similarly, a study compared the performance of MnLR, BRT and RF models for predicting water quality and found that MnLR with OA = 82% had a relative superiority over RF (78%) and BRT (74%). Moreover, the κ value was 0.78 for MnLR, while 0.62 and 0.69 for BRT and RF, respectively (Mishra et al., 2021). Therefore, based on past studies, MnLR as a prediction model of agricultural water quality class can outperform BRT and RF models. Some researchers believe that logistic regression methods can be highly effective in spatial modeling of the quality of groundwater resources due to the simplicity and speed of calculation, as well as the ability to use qualitative variables, accurate prediction, use of big data and high interpretability (Bivand et al., 2013).

3.5 Spatial distribution of agricultural water quality classes

In the next step, in order to make a better comparison, the agricultural water quality distribution map was drawn based on the simulated results using machine learning algorithms for all three models during the studied periods (Fig. 9, 10 and 11); the area related to the agricultural water quality classes for the superior model by each year is presented in Tables 8, 9 and 10.
In relation to the map prepared with the superior RF model in 2012 (Fig. 9), the results showed that most of the central, eastern and southern parts of the study area had the agricultural water quality of the Very passion class (C4-S1, C4-S2, C4 -S3 and C4-S4). In 2012, 35% of the studied area had agricultural water with C3-S1 quality in the northern, northeastern and western parts, accounting for the highest percentage of the agricultural water quality class (Table 8).
Regarding the map prepared with the MnLR superior model in 2016 (Fig. 10), the results showed that most of the central to southern parts, parts of the northeast, southwest, and east of the study area had agricultural water quality with the Very passion class (C4-S1, C4-S2, C4-S3 and C4-S4). In 2016, 52% of the studied area had agricultural water with C3-S1 quality, accounting for the highest percentage of agricultural water quality class (Table 9).
In 2020, the results showed that most of the central to southern parts, parts from the north and northeast, southeast of the studied area had agricultural water quality with Very passion class (C4-S2, C4-S3). In 2020, 44.5% of the studied area had agricultural water with C3-S1 quality, accounting for the highest percentage of agricultural water quality class (Table 10).

3.6 Groundwater elevation contour map

The groundwater elevation contour map (Fig. 12) was drawn during all three study periods to better interpret the cause of the change in agricultural water quality in the region.
The results indicated that the highest level of groundwater access was in the central to south and northeast areas in every three years (Fig. 12). In addition, the highest level of access to groundwater increased from 108 m in 2012 to 131 m in 2020, revealing the withdrawal of the groundwater aquifers in the region.
The spatial distribution maps of EC showed that the maximum value of this factor in 2020 (5203 μS/cm) compared to 2012 (4183 μS/cm) had an increasing trend. The spatial distribution maps of HCO^{3-} from 2012 to 2020 showed an increasing trend with a maximum of 4.75 mg/L in 2012, 5.60 mg/L in 2016 and 6.07 mg/L in 2020.
The percentage of the area belonging to the C4-S3 class increased from 5 in 2012 to 23.9 in 2020, indicating a decreasing trend in the water quality of the region. However, due to the increase in rainfall in 2020, the irrigation water quality class in the south of the region changed from C4-S3 in 2016 to C4-S2 in 2020; the reason for this improvement in the quality class in this area could be due to the seasonal increase in rainfall at this point, the mountainous nature of the area, and the lack of agricultural land. It should be noted that the quality of irrigation water was still in the very passion class.

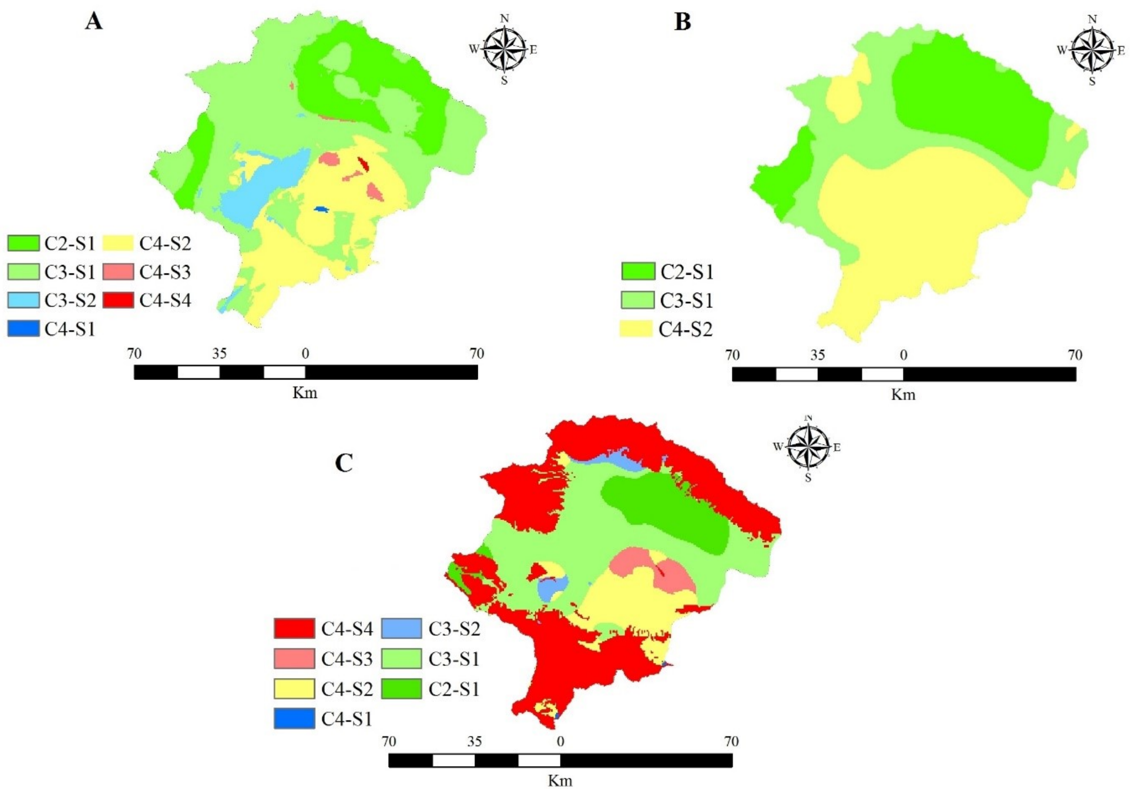

Figure 9. Spatial distribution of agricultural water quality using machine learning algorithms; (A) Random Forest, (B) Boosted Regression Tree and (C) Multinomial Logistic Regression in 2012, in Qazvin Plain, Iran.

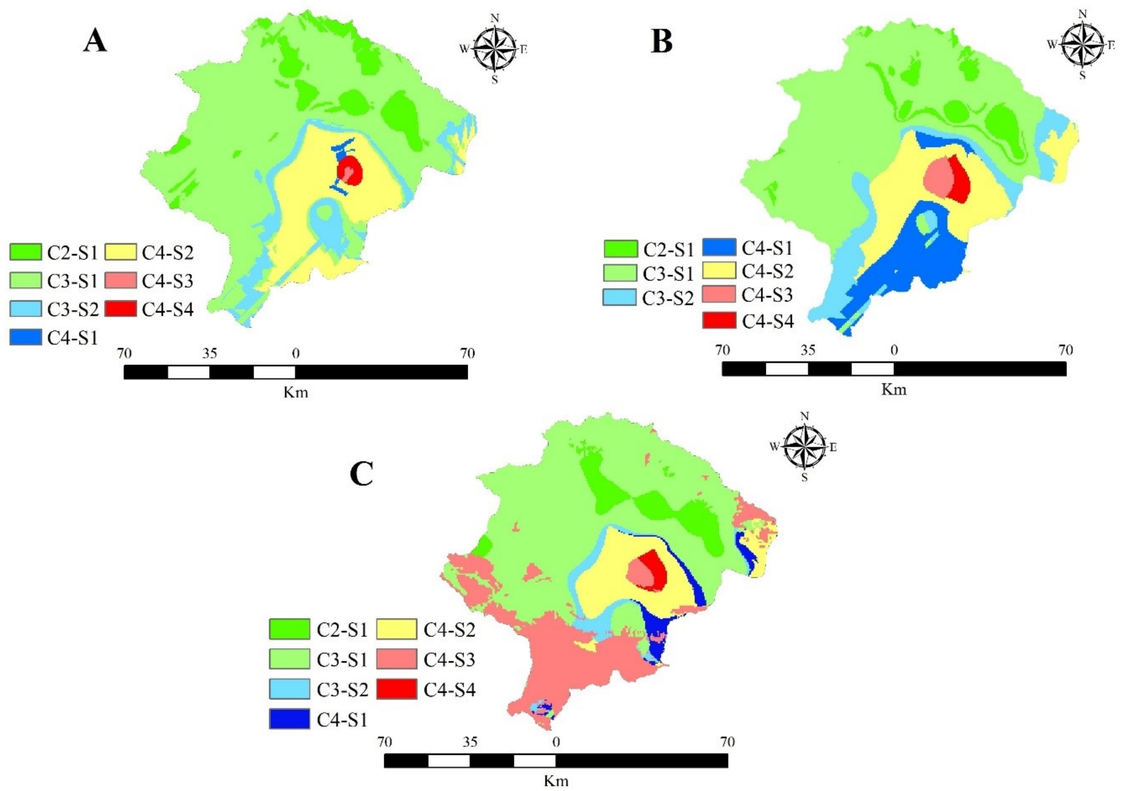

Figure 10. Spatial distribution of agricultural water quality using machine learning algorithms; (A) Random Forest, (B) Boosted Regression Tree and (C) Multinomial Logistic Regression in 2016, in Qazvin Plain, Iran.

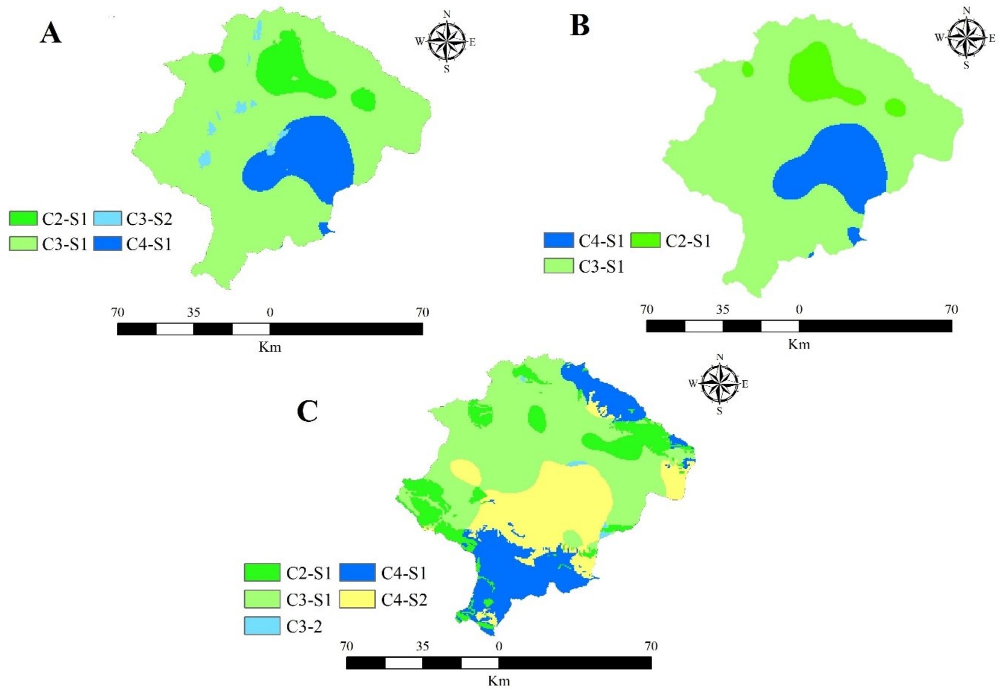

Figure 11. Spatial distribution of agricultural water quality using machine learning algorithms; (A) Random Forest, (B) Boosted Regression Tree and (C) Multinomial Logistic Regression in 2020, in Qazvin Plain, Iran.

Table 8. The area of agricultural water quality classes in 2012 based on the superior model of Random Forest in Qazvin Plain, Iran.

Classes	Area	
	Hectare	Percentage
C2-S1	19052460	20
C3-S1	33341805	35
C3-S2	14289345	15
C4-S1	952623	1
C4-S2	20957706	22
C4-S3	4763115	5
C4-S4	1905246	2
Total	952623	100

Table 9. The area of agricultural water quality classes in 2012 based on the Multinomial Logistic Regression model in Qazvin Plain, Iran.

Classes	Area	
	Hectare	Percentage
C2-S1	38371	7.21
C3-S1	495747	52
C3-S2	34526	3.62
C4-S1	27820	2.92
C4-S2	113657	11.9
C4-S3	201509	21.2
C4-S4	10634	1.12
Total	952623	100

Table 10. The area of agricultural water quality classes in 2020 based on the Multinomial Logistic Regression model in Qazvin Plain, Iran.

Classes	Area	
	Hectare	Percentage
C2-S1	125390	13.2
C3-S1	424149	44.5
C3-S2	3681	0.40
C4-S2	171767	18
C4-S3	227637	23.9
Total	952623	100

3.7 Relative importance of environmental variables

Fig. 13 shows the relative importance of predictor variables for determining agricultural water quality.

The results (Fig. 13) demonstrated that EC, HCO^{3-} and pH in 2012, 2016 and 2020 respectively, justifying about 50, 65 and 40% of the changes, were recognized as the most effective factors in determining groundwater quality, indicating the central effect of these parameters on the quality of groundwater resources for agricultural uses. Agricultural water quality is important in terms of influencing soil management and crop quality (Piri and Bamri, 2014; Bakhshandehmehr et al., 2017; Zehtabian et al., 2004), and the increase in salinity has the most negative effect on the reduction of production and productivity (Salehi Rezaabadi et al., 2020). Regarding the effectiveness of HCO^{3-} and pH parameters, the cause can be attributed to the geological features of the region. The largest area in the map of the geological formations of the study area is related to the Quaternary formations and young terraces, so that the most concentrated agricultural activities in the current conditions are also directed to these areas; it seems that Quaternary formations and young terraces have high carbonate concentration. This feature causes the groundwater from these formations to have high pH and high water hardness. These inherent features in these formations are consistent with the results of the current research and the effectiveness of these parameters in groundwater quality.

Limitation:

Parameters were selected based on data availability, relevance to regional standards, and consistency over all three time points

The selection of the 12 water quality parameters in this study was based on three main criteria: (1) data availability across all three time periods (2012, 2016, and 2020), (2) consistency with national and international guidelines for agricultural water quality, and (3) relevance to machine

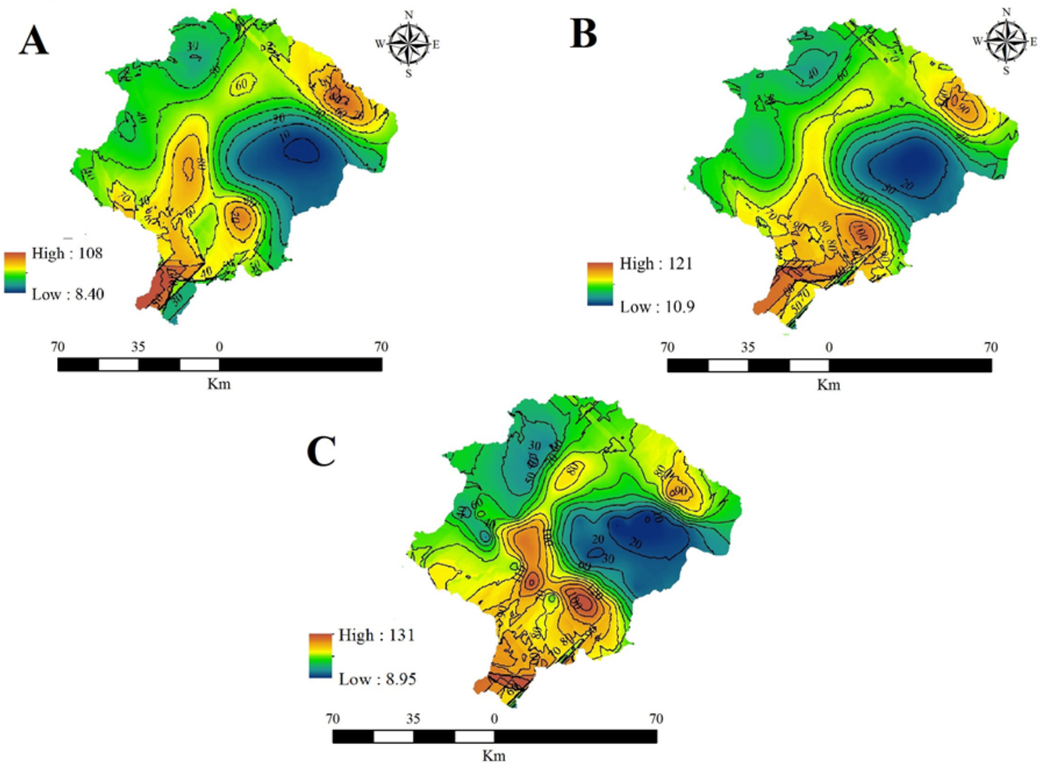

Figure 12. Groundwater elevation contour map for (A) spring 2012, (B) spring 2016 and (C) spring 2020, in Qazvin Plain, Iran.

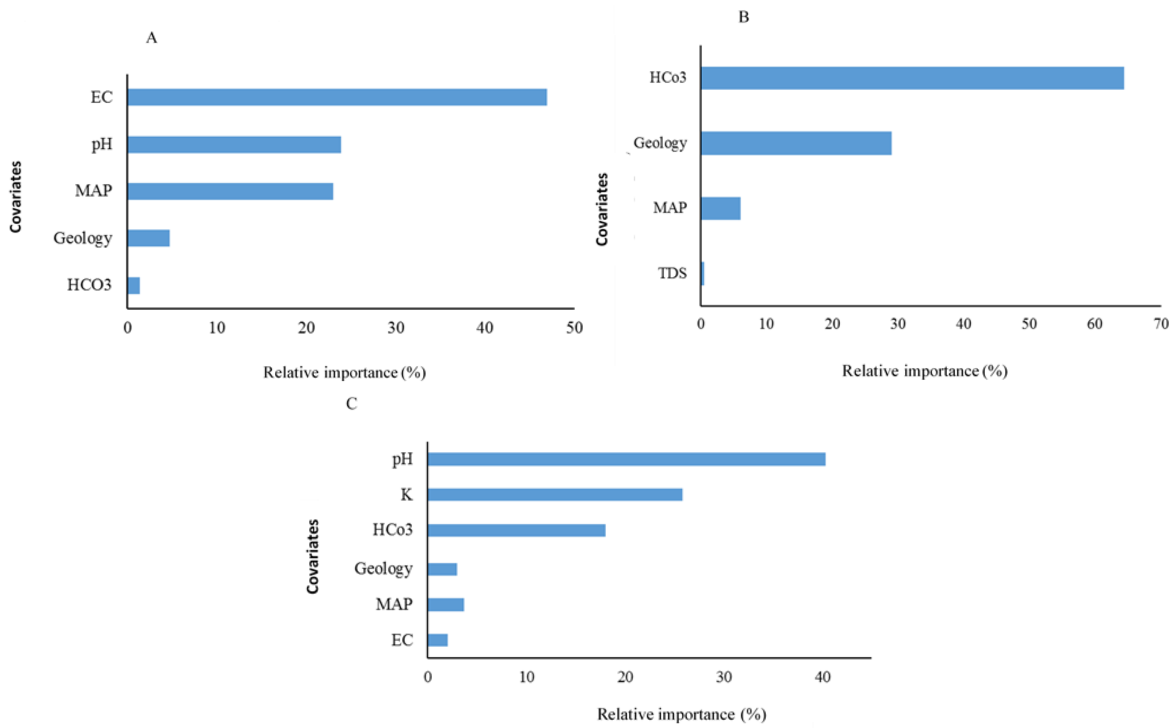

Figure 13. Relative importance of qualitative parameters and environmental variables for (a) spring 2012, (b) spring 2016 and (c) spring 2020, in Qazvin Plain, Iran.

learning classification models. Parameters such as nitrate, TSS, TOC, and organic matter were not included due to the lack of consistent, reliable data across the selected years. While these indicators are important in water quality assessment, they were excluded to ensure model consistency and comparability over time.

One of the main limitations of this study was the unavailability of some key water quality parameters, such as nitrate, total suspended solids (TSS), and organic matter, for all three time periods. Their exclusion may limit the comprehensiveness of the analysis. Additionally, the study did not directly integrate lithological or hydrogeological data into the models, which could further enhance prediction accuracy. Future studies are encouraged to address these gaps by combining geochemical and biological indicators with machine learning techniques.

4. Conclusion

The present study was conducted with the aim of investigating the effectiveness of machine learning approaches (RF, BRT and MnLR) in modeling and predicting the spatial and temporal groundwater quality classes based on the USSl diagram in the Qazvin plain, along with the introduction of the most important parameters affecting the quality of agricultural water. In addition, in order to investigate climate changes, the effect of mean annual precipitation and standardized precipitation index on groundwater quality was also studied. The results of spatial modeling in the spring of 2012 showed that the RF model had higher overall accuracy and kappa coefficient than the other two models. On the other hand, for the two years 2016 and 2020, the results indicated a higher efficiency of the MnLR model.

The trend of changes in agricultural water quality classes for all three maps showed that the percentage of the area of C4-S3 class in the central part of the region where agricultural lands are concentrated increased from 2012 to 2020, highlighting the decrease in agricultural water quality in these regions. According to the type of land use in the central areas (agriculture), increasing the level of water extraction from groundwater could be the reason for the decrease in water quality.

The groundwater elevation contour maps showed that, despite the increase in rainfall and the improvement of the drought index in 2020 in the region, the groundwater level in the central areas towards the south still had a decreasing trend, and the quality class of agricultural water in the central areas had decreased. Therefore, the amount of precipitation in the region could not compensate for the excessive exploitation of groundwater resources. In addition, this excessive exploitation could cause irreparable effects such as soil compaction, subsidence, destruction of vegetation and flood risk.

According to the land use map, parts of the east of the study area consist of barren lands with a low concentration of piezometric wells; therefore, because there is no extraction of groundwater resources, the increase in water level and better water quality was observed in the eastern regions.

The results of the relative importance of hydrogeochemical factors showed that EC, HCO^{3-} and pH were identified as the most effective parameters affecting groundwater quality in 2012, 2016 and 2020, respectively. On the other hand, the climatic factor of mean annual precipitation was not recognized as influencing factors on groundwater quality modeling.

Correspondingly, in addition to the above-mentioned results, overexploitation of groundwater resources, geological formations and land use change (anthropogenic activities) can lead to a drop in the groundwater level, salinization and subsequent soil degradation, decreased yield and ultimately the development of the desertification process.
Spatio-temporal prediction of water quality is considered a fundamental and practical ability to evaluate the process of water quality changes over time and in any geographical location, which provides basic information for monitoring and managing water quality in the study area. In this research, three widely used machine learning methods were used, which made it possible to evaluate the effect and degree of influence or the relative importance of different parameters in the state of groundwater quality, as well as to predict the spatial distribution of water quality classes in the form of a map over time. The findings of our research showed that the trend of changing water quality in different regions of Qazvin Plain during the years 2012 to 2020 has changed in an unfavorable way, which emphasizes the need to make appropriate management decisions in order to improve the conditions. Based on the findings of this study, several recommendations are proposed for water resource managers, agricultural planners, and future researchers:
For Managers and Planners:

- Implement regular spatial and temporal monitoring of agricultural water quality, especially in regions with high salinity and bicarbonate concentrations.
- Integrate machine learning-based water quality classification systems into national agricultural monitoring programs to enable early detection of degradation trends.
- Promote adaptive irrigation strategies that account for temporal changes in water quality, including crop rotation and the use of salt-tolerant crops in affected areas.
- Develop region-specific guidelines for the reuse of marginal-quality water in agriculture, supported by real-time data from monitoring networks.

For Researchers:

- Future research should integrate geological and geochemical data (e.g., lithology, sediment composition) into water quality prediction models.
- Further studies can explore the impact of climate change, land-use change, and groundwater extraction rates on water quality dynamics.
- Comparative analysis of different machine learning models across multiple basins in Iran (or globally) will improve model generalizability and reliability.
- Investigating the role of biological indicators and organic pollutants can enhance the multi-dimensional assessment of agricultural water quality.

These recommendations aim to support more sustainable water management practices and foster cross-sectoral collaboration between hydrologists, geologists, agricultural experts, and policymakers.

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Authors contributions
Authors have contributed equally in preparing and writing the manuscript.

Availability of data and materials
The data that support the findings of this study are available from the corresponding author, upon reasonable request.

Conflict of interests
The author declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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