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ORIGINAL ARTICLE

Prediction of groundwater quality in irrigated areas using a novel gradient boosting approach

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Abstract

Evaluating groundwater quality in irrigated areas is crucial for sustainable agriculture, especially as limited water resources and climate change pose significant threat to groundwater resources. Spatial information on groundwater quality is essential for effective management and utilization of water resources, particularly in intensive cropping areas such as irrigated regions in IBIS, Pakistan. However, recent advancements in machine learning (ML) techniques have highlighted that conventional groundwater quality assessment methods are costly and time-consuming, especially for developing nations. Accurate and efficient ML models can address this challenge in agricultural water management by optimally identifying the categories of water quality. This study is conducted to predict groundwater quality using an innovative ensemble-boosting methodology. The data is collected from Rahim Yar Khan's irrigation system by the Scarp Monitoring Organization. Four irrigation water quality indicators, including sodium adsorption ratio, total dissolved solids, residual sodium carbonate, and electrical conductivity, are used to predict groundwater quality by applying four ML models. The performance of the ML models is assessed using mean squared error, correlation coefficients (r), and root mean square error measures. The proposed Gradient Boosting (GB) approach combines the advantages of interpretable tree models and boosting approaches. Experimental results validate the utility of the proposed approach with a 99% accuracy in predicting groundwater quality, compared to conventional ML techniques. Based on the proposed GB model and the inverse distance weighting interpolation technique, the groundwater quality distribution in the Hazardous Area is 17.34%, the Marginal Area is 79.36%, and the Safe Area is 3.30%. Enhancement and validation of groundwater quality index predictions are carried out using k-fold validation and hyperparameter tuning. Results indicate that the ML models have the potential to accurately delineate different groundwater quality zones for managing water resources and ensuring sustainable agriculture. Water quality assessment through the proposed approach can help managing the groundwater for the regions susceptible to deterioration of water quality thus contributing to better irrigation governance.

Keywords Groundwater quality · Irrigated area · Extreme gradient boosting · Machine learning · Groundwater zoning · Artificial intelligence · Ensemble boosting

Introduction

Water supply has become crucial, particularly, in the industrial, agricultural, and domestic sectors. Improved water resource quality can lead to increased agricultural productivity while significantly reducing the cost of water treatment for irrigation. Water scarcity is thus a global issue, expected to worsen due to climate changes. In the past, water quality issues were often overlooked due to abundant high-quality water sources. Pakistan encountered significant challenges with land degradation recently, due to overexploitation and poor management of groundwater resources (Aldrees et al. 2022). Previous zoning techniques have not sufficiently addressed this problem, leading to further degradation of agricultural lands.

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Extended author information available on the last page of the article

Approximately one-third of the agricultural land in Pakistan has been degraded due to factors, like water erosion, wind erosion, soil fertility depletion, deforestation, unsustainable livestock grazing, and water logging practices (Rasool et al. 2022). The country ranks fourth globally in groundwater abstraction, extracting around 65 billion cubic meters (BCM) annually, despite having only 55 BCM of sustainable groundwater resources. This overexploitation has resulted in a significant reduction in groundwater availability, currently below 1000 cubic meters per capita annually, and is projected to decrease further to 837 cubic meters per capita by December 2025. Poor groundwater management has directly impacted crop productivity, with land degradation from salinization, water logging, and nutrient depletion leading to reduced yields and increased vulnerability to climate change. Water shortages have particularly affected farmers, closer to the end of the irrigation system, including those in Rahim Yar Khan, because of downstream theft and poor management (Dimple et al. 2022).

Pakistan has established the National Action Plan to address desertification challenges with a goal to mitigate land degradation while pursuing sustainable agricultural development. With the support of this initiative, a land policy that prioritizes resource conservation, sustainable development, and improved resource management efficiency will be created (Taşan et al. 2023). Developing new institutional frameworks, enhancing the development and management of water resources, and acquiring advanced knowledge in adaptive resource management are all essentials for these initiatives to be sustainable (Satish et al. 2024).

Research efforts have also been made in this regard. For example, El Bilali et al. (2021) examine the application of artificial intelligence (AI) models to predict water quality. They pay particular attention to how AI techniques might improve the comprehension of water quality indicators and promote effective water management. 1679 samples from various Indian states were gathered between 2005 and 2014 from specified historical places in India. The authors investigate a variety of AI approaches, such as neural networks (NN), ensemble methods, support vector machines (SVM), and decision trees (DTs). The study apparently covers the process of choosing relevant factors (pH, turbidity, dissolved oxygen, etc.) that significantly affect water quality. The authors evaluated the AI models with suitable metrics (e.g., accuracy, precision, recall, F1-score, etc.). The SVM model identifies the quality of water with a greater accuracy of 97.01%.

Kouadri et al. (2022) explored the application of ML techniques to forecasting the Water Quality Index (WQI) in the framework of the An Kim Hai irrigation system. The authors specifically look at how feature selection affects model performance and evaluate how effective ML algorithms are at identifying the quality of water. The authors figured out which four crucial factors, turbidity, TSS, DO, and Coliform, have the highest impact on the quality of the water by using the embedded technique. Based on these features, the random forest (RF) model predicts the WQI values derived from the An Kim Hai system with the maximum accuracy (94%).

Lap et al. (2023) provide a thorough evaluation of groundwater quality for agricultural use in El Kharga Oasis, within the Western Desert of Egypt. The study employed various Information Systems for Geographical (GIS) and Irrigation Water Quality Indices (IWQIs). In the research, two ML models were used, including adaptive neuro-fuzzy inference system (ANFIS) and SVM, to predict eight different indices of irrigation water quality including but not limited to Irrigation Water Quality Index (IWQI), Sodium Adsorption Ratio (SAR), Soluble Sodium Percentage (SSP), Potential Salinity (PS), Residual Sodium Carbonate Index (RSC), and Kelley Index (KI). Numerous prediction quality criteria have been employed for this research. The purpose of this study was to demonstrate that both ANFIS and SVM could successfully simulate the IWQIs, which had average coefficients of 0.76 and determination coefficients of 0.99 in the testing phase and 0.97 in the training phase. Thee obtained accuracy indicate that the models could be very helpful in predicting IWQI.

Various techniques have been reported for effective assessment of groundwater quality in irrigated regions. For conventional methods, a single index for groundwater is obtained by amalgamating several sub-indices (Li et al. 2013). This implies that these methods implicate the consideration of several parameters that contribute to groundwater quality in irrigated regions. Consequently, they are usually expensive and time consuming. Thus, it is hard to assess the quality of groundwater, especially in less affluent countries with limited resources and poor infra structure. Lately, ML algorithms have been increasingly used to assess groundwater quality. The advantage of ML algorithms is their ability to identify hidden patterns, discover the relationships in data, and accurately predict groundwater quality variables in complex situations that involve nonlinear relationships. The first step of the ML-based method for calculating groundwater quality in irrigated areas is to choose significant water quality indicators. This choice is critical as it has a significant effect on the accuracy of groundwater quality indicators.

Talukdar et al. (2022) explores the application of ML techniques to evaluate groundwater quality in irrigated areas. The research aim is to apply data-driven models to improve the comprehension of the dynamics of water quality and enable efficient oversight of water resources. Using a variety of statistical methodologies, the majority of the existing research has selected significant indicators related to water quality. In a region in Iran, the efficiency of three ML techniques, boosted regression trees (BRT), multivariate discriminant analysis (MDA), and SVM, for assessing groundwater risk was assessed. The findings show that the combination of these three models in an ensemble approach performs better than individual models. The outcome is in line with related research conducted in two different regions of Iran and Pakistan (Haggerty et al. 2023).

In this work, we introduce a novel ensemble boosting GB approach for ML-based groundwater quality prediction in irrigated areas to overcome the limitations of previous studies. The categorization of models is based on the learning approach: supervised versus ensemble methods. Less conventional or more specialized learning types, such as unsupervised and ensemble learning, have not experienced the same level of growth as supervised learning. The effectiveness of the proposed approach is validated through a case study where we evaluate groundwater quality using a dataset collected by the Scarp Monitoring Organization (SMO) in Pakistan for the Rahim Yar Khan city. The results demonstrate that the approach can significantly reduce the number of water quality factors while maintaining accuracy in groundwater quality evaluation (Majumdar et al. 2020). The following is a summary of the primary contributions of this study by using machine learning:

- A novel ensemble boosting GB approach is introduced, for predicting groundwater quality in irrigated areas. Experiments carried out on an actual dataset demonstrate that the suggested approach provides accurate predictions of groundwater quality values.
- For experiments, data was collected from Rahim Yar Khan's irrigation system by the SMO, located in the southern part of the Punjab Province, which spans an area of 1300 km^2, with a length of approximately 65 km and an average width of 20 km. It lies between longitudes 70°00 E to 70°45 E and latitudes 28°00 N to 28°45 N, with the land sloping toward the Southwest. The study area includes the canal command areas of the Abbassia and Punjnad canals.
- To identify the most significant parameters, present in the water, the effectiveness of various feature engineering approaches is investigated. In comparison to the other methods, they are more efficient and have a higher degree of impact, such that they can reduce a lot of water quality parameters for determining groundwater quality indexes.
- Experiments demonstrate that novel ensemble boosting can be an alternative to ascertain groundwater quality indices. By using these methods, analysis costs and time have been substantially reduced, and a reliable evaluation of these indicators has been made. This approach has practical applications, particularly when measuring water quality metrics, which is challenging.

The remaining manuscript, followed by sections: the next section contains the study area and materials analysis and the consequent section is based on the proposed methodology and the following section expressed the results and discussion. Finally, the last section summarizes the findings.

Study area and materials

The study is conducted using Rahim Yar Khan's irrigation system, located in the southern part of the Punjab Province, which spans an area of 1300 km^2, with a length of approximately 65 km and an average width of 20 km. It lies between longitudes 70°00 E to 70°45 E and latitudes 28°00 N to 28°45 N, with the land sloping toward the southwest. The study area includes the canal command areas of the Abbassia and Punjnad canals, as shown in Fig. 1. The canal command area of Abbassia has a Gross Command Area (GCA) of 120,739 ha and a Cultivable Command Area (CCA) of 96,139 ha. In comparison, the canal command area of Punjnad has a GCA of 613,172 ha and a CCA of 551,926 ha (Tahir and Habib 2001). This region was chosen due to its strong dependence on groundwater for irrigation and its vulnerability to water quality degradation. Wastewater from domestic, agriculture, industrial and other sources is a major contributor to pollution in within Rahim Yar Khan irrigation system. To ensure sustainable development and protect the local ecology, it is crucial to continuously monitor and evaluate water quality in this canal groundwater system (Ubah et al. 2021).

Agriculture is the primary economic activity of Rahim Yar Khan, with "Kharif" and "Rabi" being the two main cropping seasons. The total number of tube wells in Rahim Yar Khan District is 37,882. In the Abbassia canal, average water supplies remain 375 cubic meters per second in the Kharif season and 411 cubic meters per second in the Rabi season. The Punjnad Canal has a water accessibility of 536 cubic meters per second in the Kharif season and 168 cubic meters per second in the Rabi season. The main crops are millet, cotton, wheat, and sugarcane. The Indus Basin, which covers Rahim Yar Khan, is mainly composed of Quaternary alluvial deposits such as unconsolidated sands, silts and clays, forming unconfined to semi-confined aquifers that are strongly influenced by canal seepage and irrigation return flows (Qureshi et al. 2021). The groundwater is controlled by natural geochemical processes such as ion exchange between calcium, magnesium and sodium, as well as dissolution and precipitation carbonate and sulphate

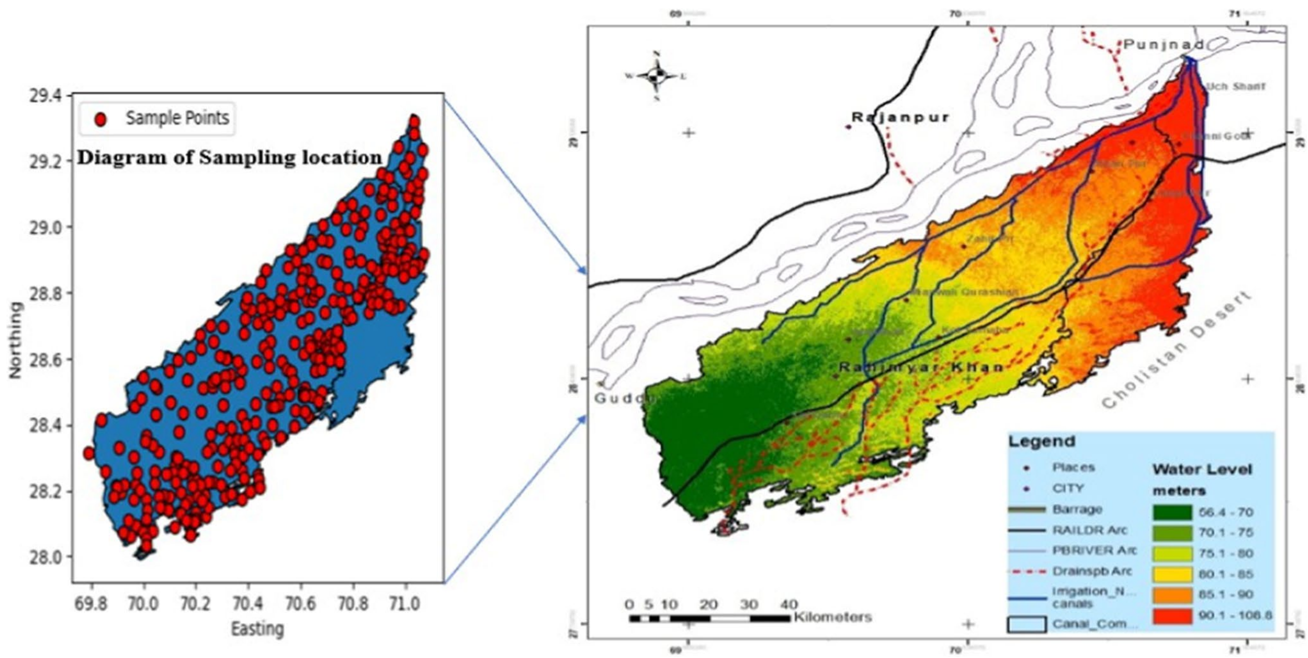


Fig. 1 Rahim Yar Khan's irrigation system and sampling locations

minerals. Irrigation effluents further intensify these reactions by mobilizing salts and nutrients, thereby altering the hydrochemical balance of the aquifer system (Ubah et al. 2021). These processes are critical in understanding the current groundwater quality and predict future risks under intensive irrigation practices.

For the lithological framework, the hydrogeological characteristics of the aquifer system are governed by hydraulic conductivity, groundwater flow regime and surface groundwater interactions. Hydraulic conductivity varies significantly with respect to the proportion of sand, silt and clay, thereby influencing aquifer transmissivity and storage capacity. The flow regime in the Indus Basin plain, including Rahim Yar Khan, is generally from the northeast to southwest, controlled by regional topography and recharge from canal irrigation. Furthermore, the interaction between surface water and groundwater plays a key role in shaping aquifer dynamics, and contributes to, both recharge and potential quality alterations through seepage and mixing processes (Ruidas et al. 2023).

Irrigation water quality's criteria

Several features, including salinity, sodicity, and toxicity, might have adverse effects on irrigation water quality. As such, it is important to evaluate and predict the chemical composition of irrigation water. Water quality criteria are determined by analyzing samples from the drainage system for parameters like electrical conductivity (EC), calcium ions (Ca^{2+}), magnesium ions (Mg^{2+}), sodium ions (Na^{2+}), carbonate ions (CO^{2-}), bicarbonate ions (HCO^{-}), as well as total dissolved solids (TDS). The outcomes are shown in Table 1. Based on these criteria, irrigation water is divided into three classes: Dangerous, Marginal, and Safe.

Table 1 Irrigation water quality standards (Punjab irrigation department)

Water quality classification	TDS (mg/L)	SAR	RSE (meq/L)	EC (μS/cm)
Useable/safe	500	0–6	0–1.25	<250
Marginal	500–700	6–10	1.25–2.5	250–750
Hazardous	>700	>10	>2.5	>750

Groundwater quality parameters

In this study, four indices of irrigation water quality: SAR, RSC, TDS, and EC, are selected and computed (Ruidas et al. 2023). These are used to determine water quality and analyze the suitability of groundwater for agricultural use within the study area (Kouadri et al. 2022).

Sodium adsorption ratio

Sodium absorption ratio (SAR) is a major factor that helps determine, if groundwater can be used for agricultural activities. It measures, how much magnesium (Mg^{2+}), calcium (Ca^{2+}) and sodium (Na^{2+}) is found in water. High sodium concentrations may cause a reduction in soil quality and disrupt groundwater balance. The calculation of SAR value involves a comparison between the amount of sodium with calcium and magnesium taken together (Kouadri et al. 2022):

$$SAR = \frac{Na^{+}}{\sqrt{\frac{Ca^{2+}+Mg^{2+}}{2}}}. \tag{1}$$

Total dissolved solids

Water is made up of many ions, which make its total ion concentration (El Bilali et al. 2021). The value of total dissolved solids (TDS) is given by the following formula:

$$TDS = \sum (cations + anions)\,. \tag{2}$$

Residual sodium carbonate

Residual sodium carbonate (RSC) is an important criterion in evaluating the suitability of groundwater for irrigation. Water chemistry and its usability for irrigation largely depends on the amount of bicarbonates and carbonates. High concentrations of carbonates and bicarbonates, compared to those made up of calcium or magnesium, result in a poor quality of water (Kouadri et al. 2022). The RSC value for a given type of groundwater can be determined using the following equation:

$$RSC = \left(HCO_3^- + CO_3^{2-}\right) - \left(Ca^{2+} + Mg^{2+}\right). \tag{3}$$

Electrical conductivity

In irrigation regions, electrical conductivity (EC) is one of the most important indicators to gauge how good or bad the groundwater is. It indicates how much dissolved salt will affect crop yields and soil health. EC can be calculated using Eq. 4:

$$EC = \frac{Total\ Dissolved\ Solids(TDS)}{Volume\ of\ Water}. \tag{4}$$

Ionic concentrations are measured in milliequivalents per liter (meq/L); this is because TDS is normally expressed in milligrams per liter (mg/L) (El Bilali et al. 2021).

Proposed methodology

The purpose of this section is to describe the proposed method for estimating ground-water quality in irrigated lands. A comprehensive analysis of the proposed approach is also provided. Figure 2 presents the architectural view of the proposed approach. The analyses are based on Rahim Yar Khan groundwater quality metrics obtained from the Pakistani Scarp Monitoring Organization (SMO) 2022 dataset. The original contains high dimensional feature set. To deal with this issue, a new feature engineering strategy is adopted that retains features with a great impact on groundwater quality prediction. The dataset is divided into subgroups used for testing (30%) and training (70%). This is followed by training and testing different state-of-the-art models. The performance of hyperparameter-optimized models is evaluated on the unseen test data. Finally, the proposed approach is used to predict groundwater quality in irrigated areas (Aldrees et al. 2022).

Phase A: novel dataset collection

For experimental evaluation, the number of samples from each groundwater source was determined using stratified sampling approach to ensure representative spatial coverage. The dataset obtained from SCARP Monitoring Organization, consists of 341 samples collected from various wells across the study area. Sampling criteria included aquifer characteristics, proximity to surface water, accessibility and statistical robustness for machine learning modeling. The dataset includes attributes related to groundwater, including residual sodium carbonate (RSC), EC, TDS, and sodium adsorption ratio (SAR).

There are approximately 341 records in this dataset that are classified as Hazardous, Marginal, and Safe. The inputs for models include EC, RSC, TDS, and SAR features. The outputs of the models include three classes of groundwater

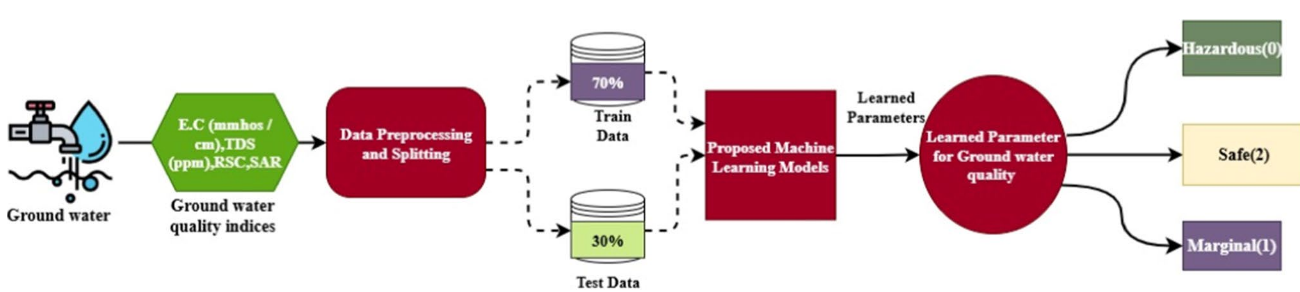


Fig. 2 Architecture analysis of proposed research methodology

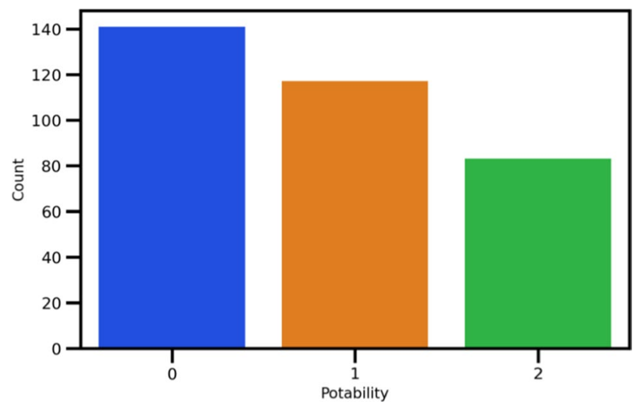


Fig. 3 The groundwater quality prediction analysis's target distribution analysis

quality prediction indices: 0 (hazardous), 1 (marginal), and 2 (safe), as shown in Fig. 3.

We present the distributions (histograms) of each parameter in Fig. 4 to improve comprehension of the collected data and provide insights into the range and frequency of values (El Bilali et al. 2021). Furthermore, line graph in Fig. 5 illustrate trends and changes in the parameters over a specified period.

Phase B: data preprocessing

Data preprocessing is an important stage in machine learning as far as predicting groundwater quality is concerned. The unprocessed data must be transformed into a better-suited form for machine learning. This procedure should also simplify the inconsistencies and missing values that

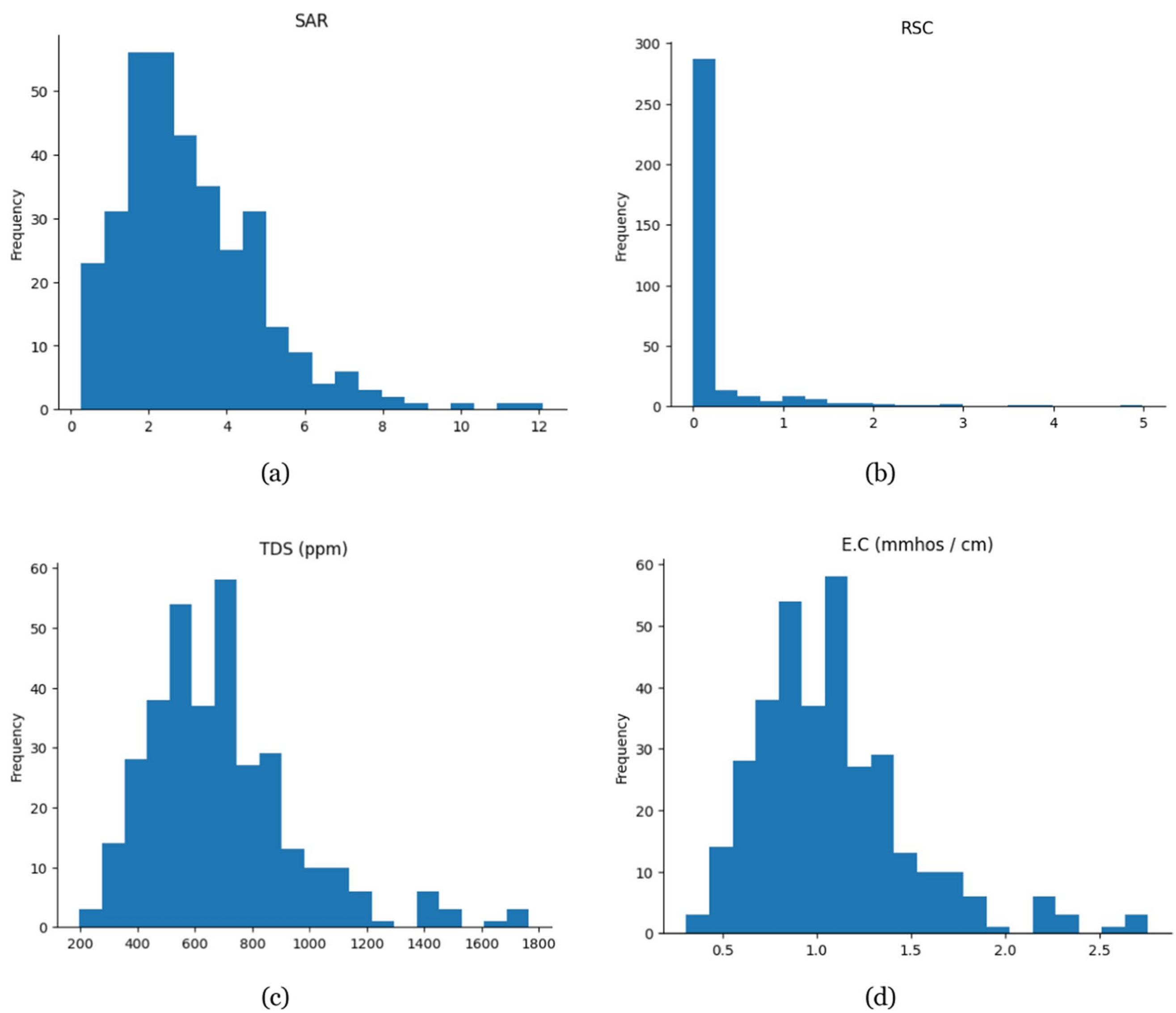


Fig. 4 The distributions analysis of the dataset

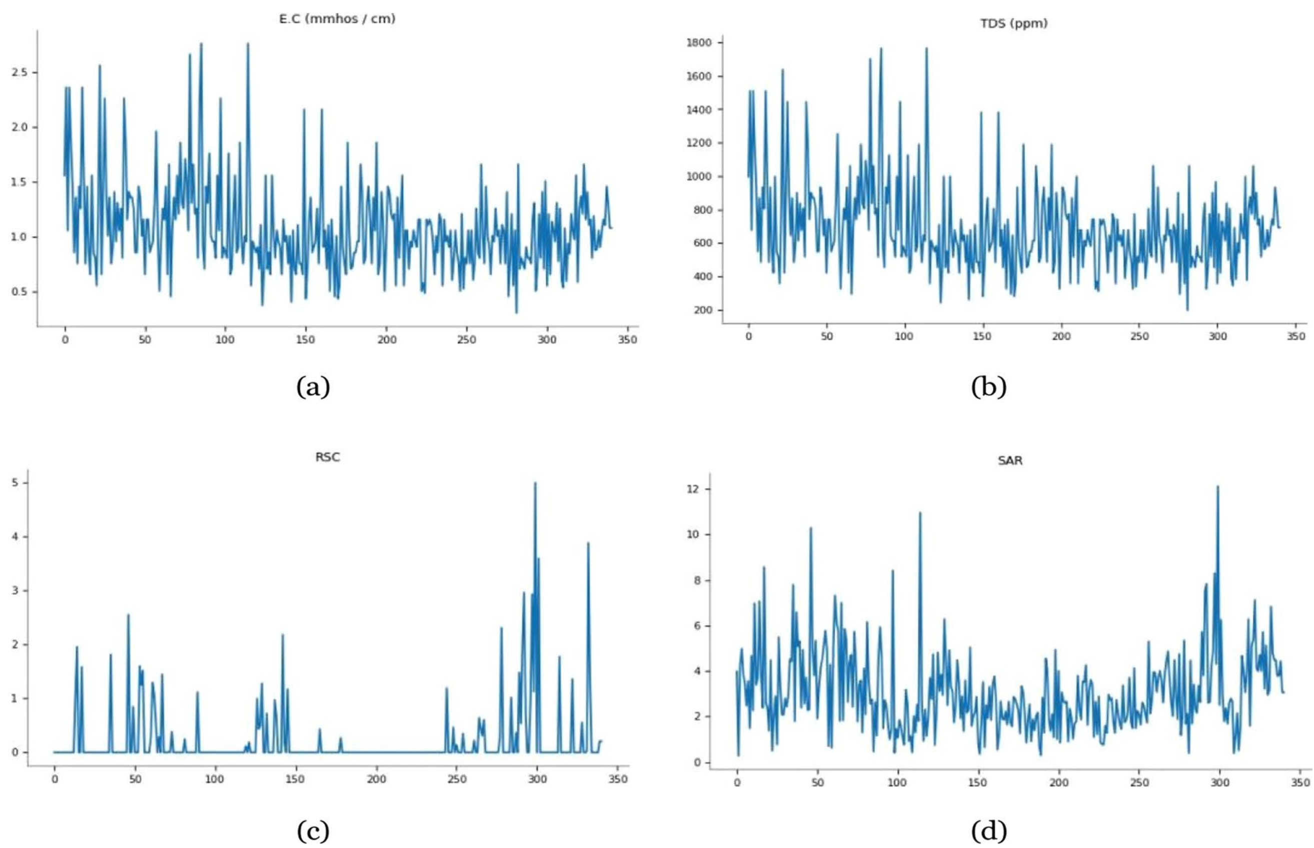


Fig. 5 The line graphs of values over time

would lower prediction results. Mean imputation (which replaces absent cells with their respective column averages) ranks among the commonly used methods for preparing data for machine learning models. It helps machine learning algorithms by maintaining consistent numerical formats hence allowing for easy understanding and interpreting (Bedi et al. 2020).

To further analyze the data, a correlation analysis is carried out. The resulting correlation matrix is shown in Fig. 6 which is good at providing insights into relationships of various factors (attributes) of the dataset. The correlation coefficient of approximately 0.96 between TDS and EC parameters indicates a very strong positive association. The correlations between RSC and TDS range from 0.70 to 0.94, indicating a moderate to substantial relationship. There is little to no correlation between EC and RSC, with the coefficient being nearly zero. Similarly, there is no discernible linear relationship between TDS and RSC or SAR. These values collectively illustrate the correlation of various water quality measures. Understanding these associations aids in predicting groundwater quality, evaluating soil hazards, and making informed decisions in agriculture, environmental science, and water management (Islam et al. 2021).

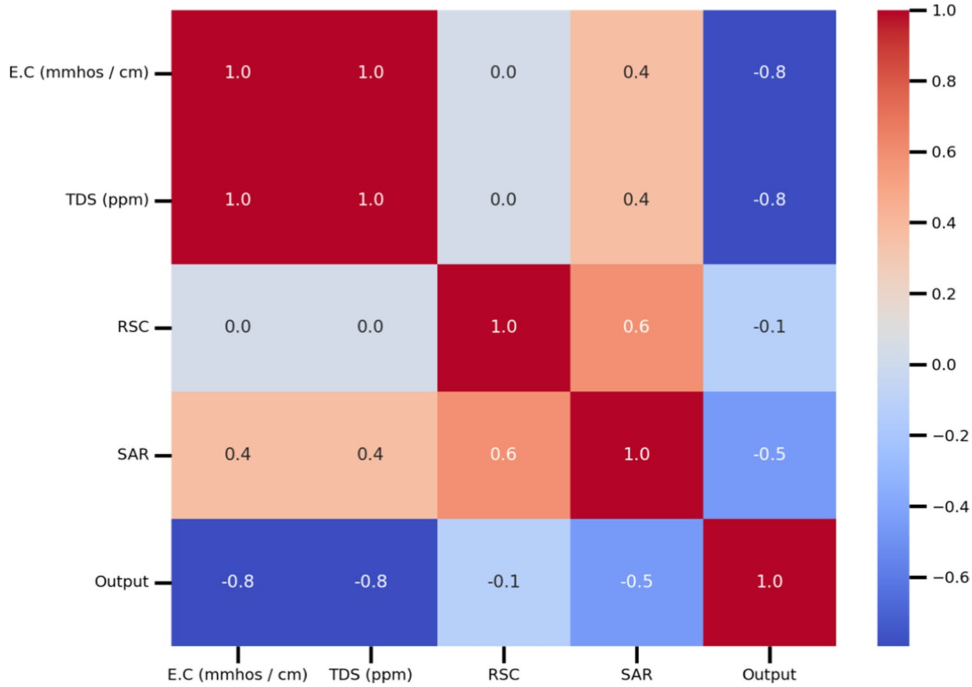
Phase C: dataset splitting ratio

By employing data splitting, we reduce the probability of model overfitting, ensuring that the trained model performs effectively on the unseen test data. For machine learning classifiers, we divide the groundwater quality indicators dataset into training and testing subsets (El Bilali and Taleb 2020). A 70% of the data is allocated for training and 30% for testing, enabling us to generate findings on the unseen data. The applied classifiers are highly accurate, and well-trained.

Phase D: applied artificial intelligence method

The purpose of data splitting is to prevent issues such as model fitting and to enhance groundwater quality assessment. Recent advancements have shown great promise in integrating AI approaches for predicting groundwater quality indices in irrigated areas. This approach leverages advanced deep-learning models and computer vision techniques to facilitate precise and real-time analysis of groundwater quality indices (Elbeltagi et al. 2022). The AI-driven systems offer valuable insights to aid farmers and other stakeholders in making informed decisions about irrigation

Fig. 6 Correlation matrix of groundwater quality prediction



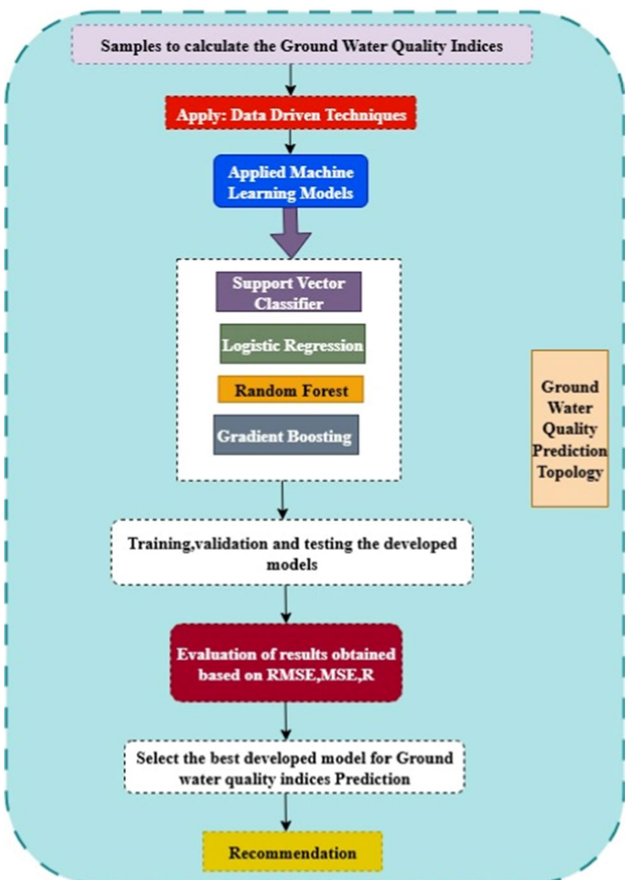


Fig. 7 Flow chart of the methodology of groundwater quality prediction

water quality. In this study, four models are utilized to predict groundwater quality needs, as illustrated in Fig. 7.

- **Logistic Regression** Logistic regression (LR) is one of the commonly used probabilistic statistical models for classification problems. While working best with linearly separable data, it has a tendency to overfit high-dimensional datasets. Overfitting can be avoided using regularization methods like L1 and L2. A major advantage of LR is its assumption of linearity that exists between dependent and independent variables. LR predominantly serves as a classification tool, yet can also be used for regression problems. The LR model is defined by the following equation:

$$LR = \frac{1}{1 + e^{\{-(\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_n x_n)\}}} \quad (5)$$

where β_0 represents the intercept, β_1, β_2, …, β_n are the coefficients for the predictor variables x_1, x_2, …, x_n, and e denotes the base of the natural logarithm. This model is used to forecast the probability of occurrence of a binary event, such as whether or not a particular water quality parameter exists, using the predictor variable values.

- **Random Forest** Among the most recognized machine learning models in is the random forest (RF), which has numerous uses in data science. It involves 'parallel ensembling' where different subsets of data are used to concurrently train various decision tree classifiers. Ultimately, it either averages them or uses majority voting for the final output. Consequently, this procedure reduces the chances of overfitting while at the same time improving predictive accuracy and supervision. Therefore, compared to single decision tree models, multiple decision trees forming a RF model are generally more accurate. This model can produce reliable results regardless of whether the variables involved are continuous or categorical. Hence, it is applicable in regression, as well as classification problems (Elzain et al. 2024). The RF model can be mathematically represented as follows:

$$RF = \frac{i}{n}\sum_{i=1}^{n}\left(\frac{\sum_{j=1}^{m} w_{ij}\cdot f_{ij}}{\sum_{j=1}^{m} w_{ij}}\right) \tag{6}$$

where n denotes the amount of decision trees, m represents the number of attributes, w_{ij} refers to the weight allotted to the jth attribute in the ith decision tree, and finally f_{ij} indicates the prediction derived from the jth attribute in the ith decision tree.

- **Support Vector Classifier** Support vector classifier (SVC) is a popular machine learning classification technique for tasks like groundwater quality prediction (Elzain et al. 2023). The main idea behind it is support vectors, which are points closest to the decision boundary in the dataset. Essentially, the SVC operates as a maximum margin classifier, aiming to maximize the separation between different classes. The SVC formula is expressed as:

$$SVC = sign\left(\sum_{i=1}^{n}\alpha_i y_i K(x_i, x) + b\right) \tag{7}$$

where α_i represents the Lagrange multipliers, y_i denotes the class labels, $K(x_i, x)$ signifies the kernel function, and b stands for the bias term. In the realm of ground-water quality prediction, SVC proves valuable for categorizing water samples based on diverse parameters including pH, EC, DO, and turbidity.

Table 2 Hyperparameters description of applied machine learning models

Technique	Hyper parameter description
LR	(random state = 1, solver = lbfgs, max iter = 100, multi class = auto, C = 2.1)
RF	(n estimators = 3, max depth = 1, random state = 0, criterion = entropy)
SVC	(random state = 0, max iter = 300)
GB	(random state = 2, n estimators = 10, learning rate = 0.1, max depth = 7)

- **Gradient Boosting** Gradient boosting (GB) stands as a robust machine learning algorithm, combining numerous week models, predominantly decision trees, to forge a potent predictive model. Demonstrating efficacy in groundwater quality classification, GB emerges as a promising technique within this domain. The GB formula is expressed as:

$$GB = \sum_{i=1}^{m}\gamma_i h_i(x) \tag{8}$$

where M denotes the number of decision trees, γ_i represents the learning rate, and $h_i(x)$ signifies the prediction of the ith decision tree. The GB algorithm operates by iteratively incorporating new decision trees to the model. Each tree aims to rectify errors made by preceding trees. This iterative process persists until the model achieves maximal performance (Gaagai et al. 2023).

Phase E: model hyperparameter settings

When developing a predictive model for groundwater quality in irrigated areas, choosing the appropriate hyperparameters is essential to obtain optimal output. These choices have a significant impact on the model's efficacy, robustness, and generalization capacity (Haggerty et al. 2023). Hyperparameter configuration for the used models is given in Table 2.

Phase F: model's evaluation criteria

Several performance indicators can be used to assess the efficiency of the machine learning models (Dimple et al. 2022).

Root mean squared error

The root mean squared error (RMSE) is the square root of the mean squared error (MSE); therefore, they are similar. This square root process yields RMSE, a measure that can help in ascertaining the stability of the accuracy metric. It also shows the standard deviation of errors (Dimple et al. 2022):

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{N}\left(Q_A^{\{i\}} - Q_p^{\{i\}}\right)^{\{2\}}}. \tag{9}$$

Mean squared error

MSE like mean absolute error (MAE) computes the squares of differences between actual and predicted values, rather than finding the actual figures. The squared deviation highlights the largest discrepancies making them even more prominent. With this metric, the total error can be calculated with greater precision and large errors will be considered more deeply (Dimple et al. 2022). MSE can be calculated using the following equation:

$$MSE = \frac{\sum_{i=1}^{n} \left(Z_i - Z^i\right)^2}{n}. \tag{10}$$

Coefficient of correlation

To assess how well the experimental data aligns with the model, we calculate the coefficient of correlation (r) using the following equation:

$$r = \sqrt{1 - \frac{\sum_{i=1}^{n} \left(Z_i - Z^i\right)^2}{\sum_{i=1}^{n} \left(Z_i\right)^2}} \tag{11}$$

where n is the total number of variables, Z_i/P_i are the observed values against which the model predicts, and Z'/M_i are the computed values (Dimple et al. 2022).

Results and discussion

In this section, we provide an in-depth evaluation of the machine learning techniques to predict water quality in cultivated regions. We present a detailed examination of the research's results and explore their implications. The outcomes indicate how precise and effective machine learning models can be to predict water quality Ibrahim et al. (2023).

Experimental setting

We applied several machine learning models using Python 3.0 to forecast the quality of underground water. Experiments are conducted using Google Colab, an open-source platform that features a GPU backend, has 13 GB RAM, and 90 GB of memory size. The metrics used for the evaluation of groundwater quality forecasts included recall, precision, accuracy, F1 score, and runtime computation (Al-Sultani et al. 2021).

- **Accuracy:** One of the striking features of classification algorithms is their accuracy which is considered as a standard evaluation measure. It is defined as a ratio of correctly categorized samples to all the predicted samples:

$$Accuracy = \frac{Number\ of\ correct\ predictions}{Total\ number\ of\ predictions}. \tag{12}$$

- **Precision:** Precision provides a quantitative measure of the performance of the model. It relates to the fraction of data samples that the model correctly predicts as positive. The formula for precision is the number of true positives divided by the overall sum of true positive and false positive values:

$$Precision = \frac{True\ Positives}{True\ Positives + False\ Positives}. \tag{13}$$

- **Recall:** Recall denotes the percent of positive samples that are correctly predicted by the machine learning model. Recall is calculated using total true positives divided by the false negatives and true positives:

$$Recall = \frac{True\ Positives}{True\ Positives + False\ Negatives}. \tag{14}$$

- **F1 Score:** F-score or F-measure, measures the accuracy and recall of an algorithm. F-score refers to the harmonic mean of recall and precision:

$$F1\ Score = 2 \times \frac{Precision \times Recall}{Precision + Recall}. \tag{15}$$

Performance analysis of applied machine learning models

This section presents a performance analysis using all features to predict groundwater quality in irrigated areas. Each model is evaluated using the complete dataset, and results are given in Table 3. The assessment parameters included accuracy, precision, recall, and F1 score, along with an analysis of the classification report. The results indicate that machine learning models generally outperform deep learning methods.

The SVC method had the lowest accuracy of 43%. SVC model does not heavily depend on the choice of network architecture and are less susceptible to overfitting due to the absence of iterative training processes. They also generally offer faster performance (Masroor et al. 2023). However, SVC still depends on the selection of kernel functions, which can influence the results as different kernels map data into higher-dimensional spaces differently. Thus, researchers should anticipate that results from these models are

Table 3 Performance metrics analysis results for applied machine learning models

Method	Accuracy	Target class	Precision	Recall	F1
RF	0.74	Hazardous (0)	1.00	1.00	1.00
		Marginal (1)	0.54	1.00	0.70
		Safe (2)	0.00	0.00	0.00
		Average	0.60	0.74	0.65
LR	0.98	Hazardous (0)	1.00	0.95	0.98
		Marginal (1)	0.94	1.00	0.97
		Safe (2)	1.00	1.00	1.00
		Average	0.98	0.98	0.98
SVC	0.43	Hazardous (0)	0.43	1.00	0.60
		Marginal (1)	0.00	0.00	0.00
		Safe (2)	0.00	0.00	0.00
		Average	0.18	0.43	0.26
GB	0.99	Hazardous (0)	1.00	1.00	1.00
		Marginal (1)	1.00	1.00	1.00
		Safe (2)	1.00	1.00	1.00
		Average	1.00	1.00	1.00

Table 4 Applied ML models performance testing

Parameters	Statistical indices	LR	RF	SVC
E.C (mmhos/cm)				
RMSE	1.18	0.97	0.43	1.18
MSE	1.39	0.94	0.19	1.39
R	0.974004	0.871596	0.09261	1.00
TDS (ppm)				
RMSE	730.74	730.88	730.37	730.74
MSE	533,957.86	534,179.48	533,435.16	533,435.16
R	0.974004	0.871596	0.09261	1.00
RSC				
RMSE	1.23	0.84	0.97	1.21
MSE	1.51	0.70	0.95	1.47
R	0.974004	0.871596	0.09261	1.00
SAR				
RMSE	3.18	3.20	2.73	3.18
MSE	10.11	10.22	7.44	10.12
R	0.974004	0.871596	0.09261	1.00

highly dependent on specific model configurations and are context-specific rather than universally applicable.

In comparison, RF demonstrated superior performance, with an accuracy of 74%. The GB model achieved an impressive 99% accuracy, followed by the LR model which demonstrated a 98% accuracy (Mohseni et al. 2024).

Table 4 displays the performance metrics for various models in determining EC, TDS, SAR, and RSC. A detailed confusion matrix analysis, illustrated in Fig. 8, is also given to assess the effectiveness of the different models. The analysis showed that the LR, SVC, and RF models exhibited high error rates for target classes when utilizing the original features, suggesting less effective classification performance (Mosavi et al. 2020). Conversely, the GB model demonstrated notably lower error rates for target classes, as indicated by its confusion matrix.

These findings emphasize the importance of meticulously selecting appropriate features and classification techniques to achieve optimal results. The study indicates that ensemble learning-based feature engineering is essential for further enhancing the performance of machine learning models on this dataset. A histogram-based bar chart analysis, depicted in Fig. 9, is used to present the performance of various machine learning models.

Model's evaluation criteria for training data

Prior to the training phase, the data are arranged in CSV files and partitioned into two sets: 239 samples for training and 102 samples for testing. To mitigate the risk of model overfitting, k-fold cross-validation with (k = 10) is utilized for training (Omeka 2023). The optimal architectures, functions, and hyperparameters for each model are established through iterative experimentation and adjustments during the training phase. Table 5 shows the RMSE, MSE, and r values of the models during the training process. As shown in Table 5, and Fig. 10 the GB model demonstrated the best results with an RMSE and MSE of 0.00, along with an r-value of 1.00, indicating the best prediction accuracy. In contrast, the LR model had an RMSE of 0.18, MSE of 0.03, and r value of 0.97, showing good but slightly lower performance. The RF model had an RMSE of 0.51, MSE of 0.21, and r value of 0.87, while the SVC model showed the poorest performance with an RMSE of 0.81, MSE of 1.19, and r value of 0.09.

Model's evaluation criteria for testing data

Following the training phase, each model is tested using 102 samples for performance evaluation in the testing phase. Results of the models evaluated are represented in Table 6 with their RMSE, MSE, and correlation coefficient (r) values. Performance metrics for each model are shown in Fig. 11. According to the RMSE of 0.31, MSE of 0.10, and r value of 0.97 achieved by the LR model, it can be said that it shows good performance. On the other hand, the SVC showed RMSE, MSE, and r values as 0.83, 0.69, and 1.00, respectively, while RF presented an RMSE equal to 0.50, an MSE equal to 0.25, and an r value equal to 0.88. The GB model shows the best performance with the best prediction accuracy, an RMSE of 0.00, an MSE of 0.00, and an r value of 1.00. Based on these measurements, it can be concluded that the GB model outperformed other models during (Pandya et al. 2024).

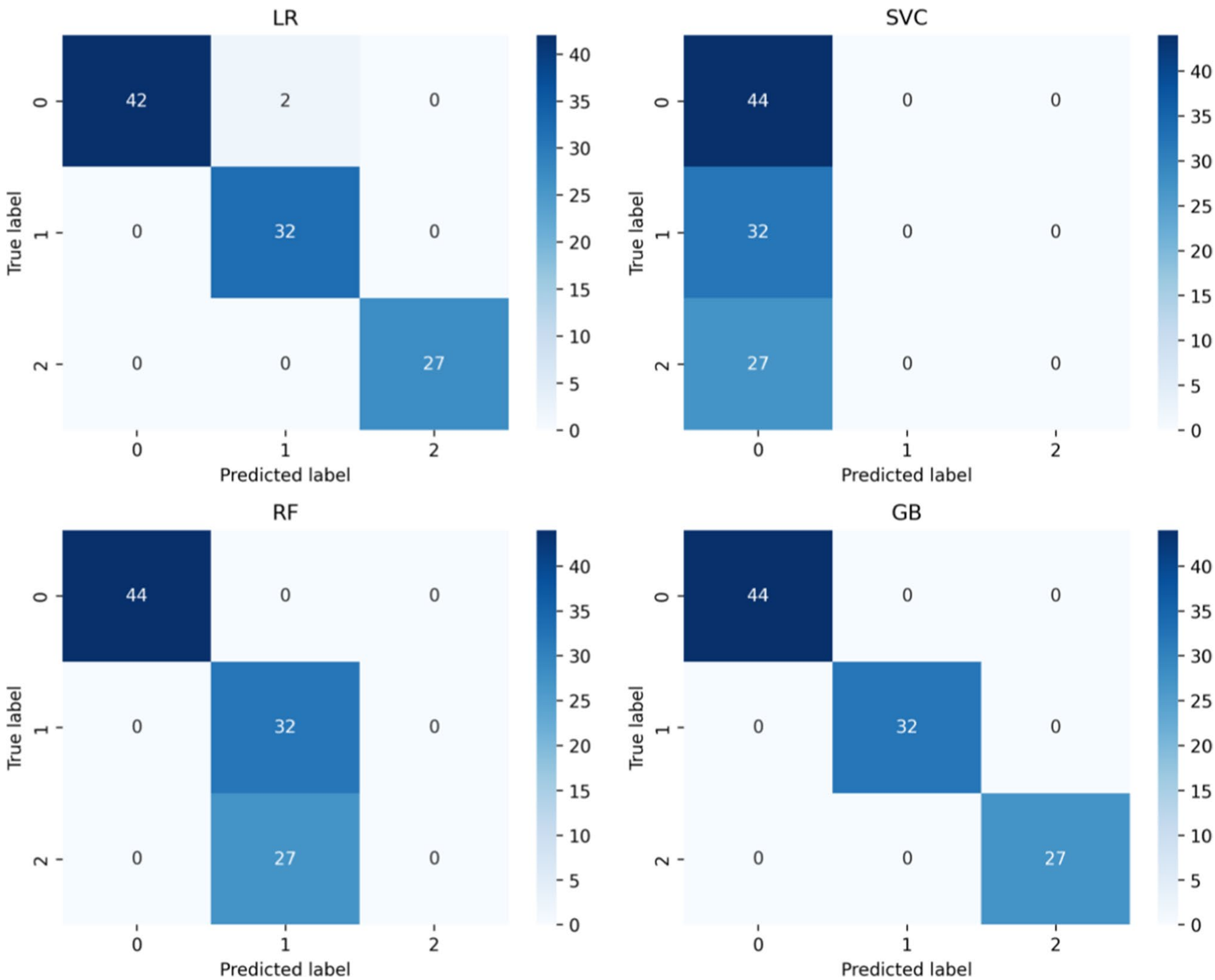


Fig. 8 Confusion matrix of applied machine learning models

Fig. 9 Histogram-based bar chart analysis of applied machine learning models

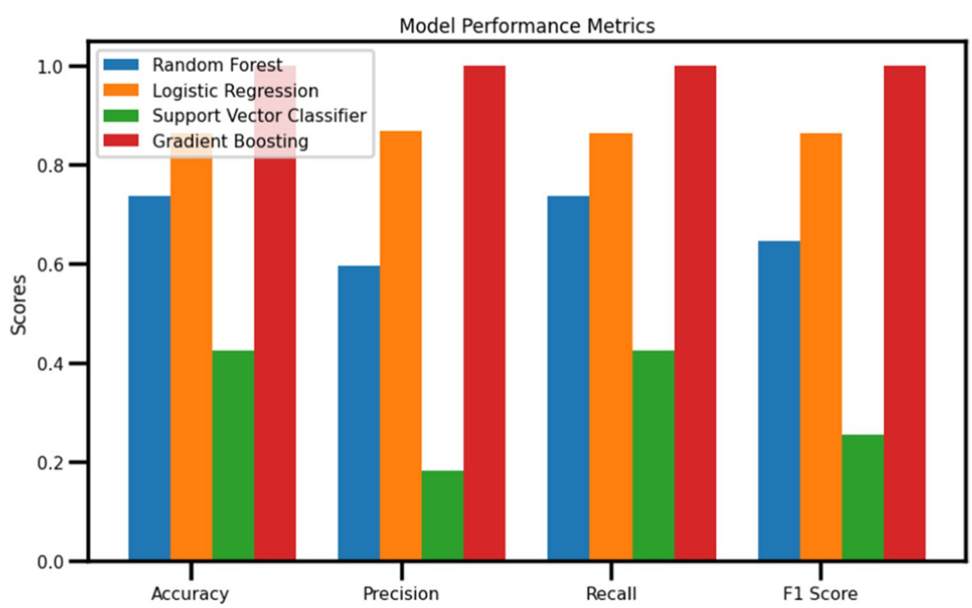


Table 5 RMSE, MSE, and *r* values of the different ML models during the training process

Model Name	RMSE	MSE	r
LR	0.18	0.03	0.97
SVC	0.81	1.19	0.09
RF	0.51	0.21	0.87
GB	0.00	0.00	1.00

Table 6 RMSE, MSE, and *r* values of the models during the testing phase

Model name	RMSE	MSE	r
LR	0.31	0.10	0.97
SVC	0.83	0.69	1.00
RF	0.50	0.25	0.88
GB	0.00	0.00	1.00

K-fold cross-validation

Table 7 shows the results of k-fold cross-validation to assess the performance of the models. The process involved computing standard deviations and k-fold accuracy as a means of validation. For this purpose, the dataset was divided into ten equal subsets. The findings show that during validation, better validation scores are obtained with the machine learning models (Pham et al. 2022). In particular, the GB model showed a low standard deviation of 0.0088 and an astonishing k-fold accuracy score of 0.997. This suggests that the GB model can be potentially used for accurate prediction of groundwater quality in irrigated areas.

Proposed gradient boosting approach

Ensemble models are quite effective in forecasting the quality of groundwater. Research shows that combining convolutional neural networks (CNNs) with other machine learning approaches and ensemble fuzzy models significantly improves predictive accuracy (Qureshi et al. 2021). By merging multiple models, ensemble techniques overcome the limitations of single models and generate more accurate results. Of the literature, only 10% and 7% focus on ensemble learning methodologies, with most studies focusing on supervised models. Supervised models are most commonly used in groundwater quality modeling, and GB has shown better performance.

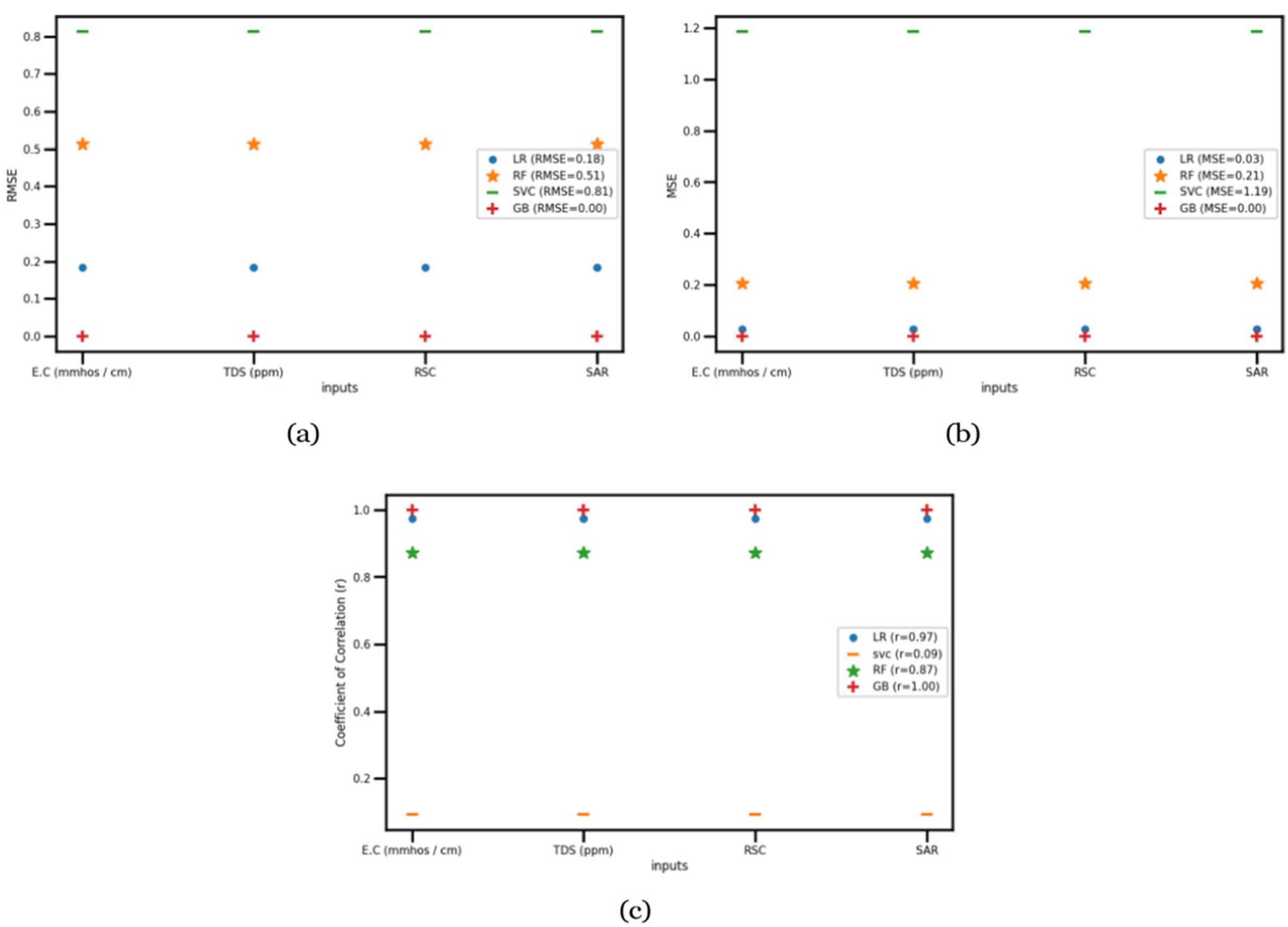


Fig. 10 RMSE, MSE, R of applied models for training data

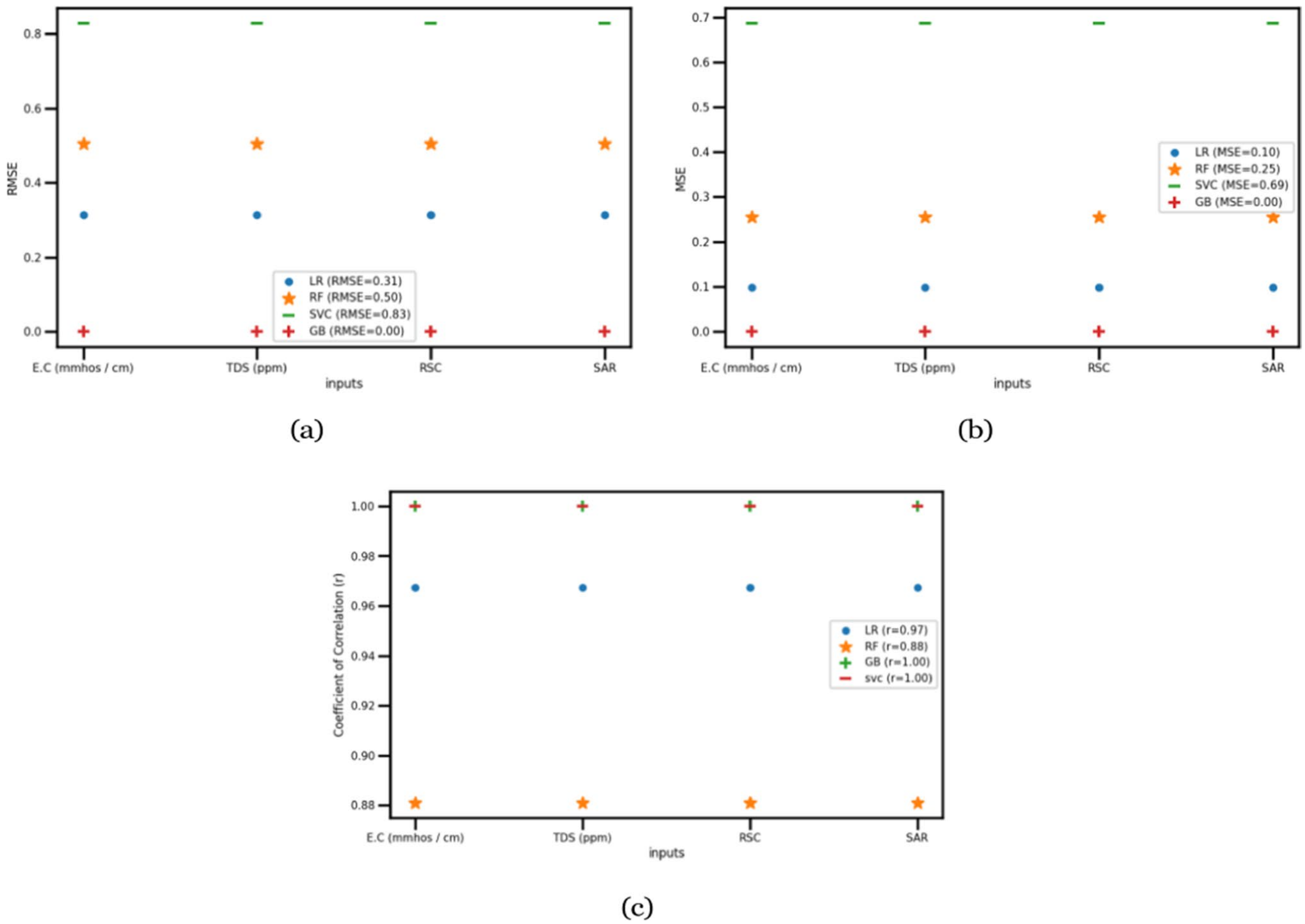


Fig. 11 RMSE, MSE, R of applied models for testing data

Table 7 Implementation of K-fold cross-validation for evaluating and enhancing the performance of machine learning models

Method	K-fold accuracy	Standard deviation
RF	0.7676	0.1048
LR	0.982	0.0195
SVC	0.3401	0.1106
GB	0.997	0.0088

The GB is an ensemble boosting technique developed to improve groundwater quality predictions in irrigated areas. This technique leverages the strengths of various machine learning algorithms to deliver more accurate groundwater quality forecasts. The ensemble model combines predictions from LR, GB, and RF models, leading to a more thorough and reliable assessment of groundwater quality. The model's effectiveness is highlighted by its precision score of 0.9708 and cross-validation accuracy of 0.997 (Raheja et al. 2024). The computation runtime was recorded, with the training phase requiring only 0.037 s and the prediction phase completed for all the samples within less than 1 s. Whereas, conventional groundwater quality assessment rely on interpolation techniques and hydrogeochemical analyses which are labor intensive, time consuming lower predictive accuracy (Arkoc 2022; Li et al. 2013); ; . Similar findings have been reported in recent studies where machine learning methods significantly outperformed traditional groundwater assessment techniques in term of efficiency and accuracy (Aldrees et al. 2022).

Moreover, this method can accurately forecast essential groundwater quality indicators such as TDS, EC, SAR, and RSC. These indicators are vital for ensuring the safety of irrigation water. By locating areas with poor water quality, the proposed approach supports the management of groundwater in irrigated regions and offers valuable insights to decision-makers for better resource management and preservation.

Extreme gradient boosting

As an ensemble learning approach, boosting is the general technique that reduces the variance during each base model's evaluation by changing sample weights iteratively to minimize the overfitting probability. According to Salem et al. (2023), extreme gradient boosting (XGBoost) outperforms

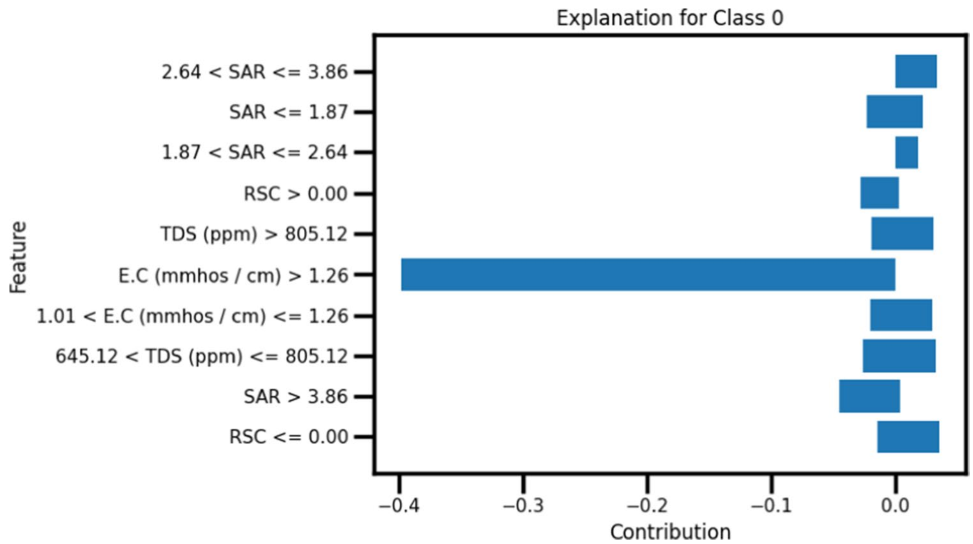


Fig. 12 Negative class explanations

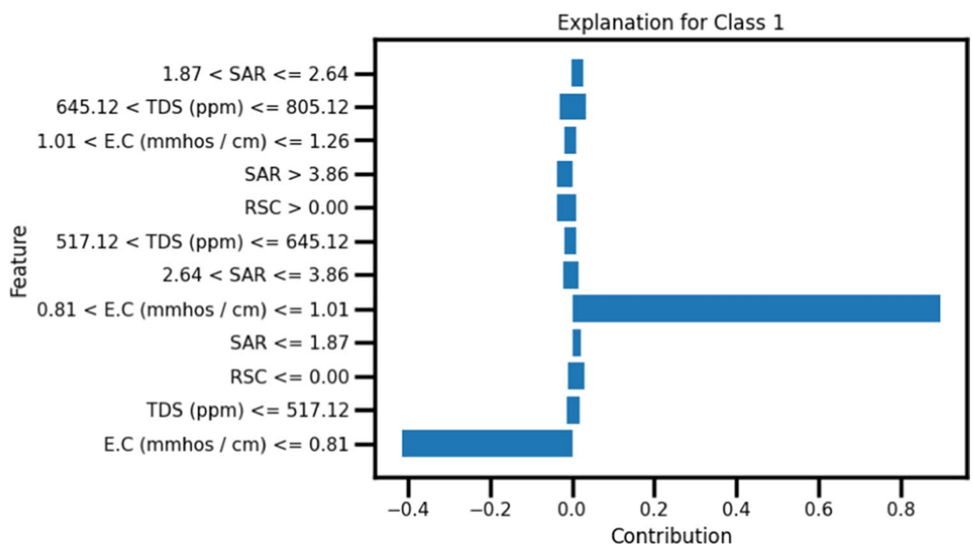


Fig. 13 Positive class explanations

deep neural networks (DNN) and MLR in groundwater salinity mapping. A unique version of gradient boosting that specifically uses regularization to enhance model generalization is called XGBoost. It has been found that using XGBoost for groundwater vulnerability prediction framework is superior to some models, such as AdaBoost, RF, LGBM, and categorical boosting (CatBoost). Accurate prediction of groundwater quality is very important for sustainable water management, especially in areas relying on irrigation. The complicated relationships in various attributes of groundwater quality are well captured by XGBoost, and its feature importance scores are useful in identifying the most significant ones. Research indicates that XGBoost gives better results than ANN, DNN, and MLR in predicting nitrate levels, salinity levels, and pesticide presence in underground water sources while performing almost parallel to SVM.

For negative class predictions (Class 0), a bar graph in Fig. 12 illustrates the contribution of various features. Each feature's importance is shown by the height of its corresponding bar. The most influential feature for predicting Class 0 is EC. When EC (measured in mhos/cm) exceeds 1.26, it strongly indicates poor groundwater quality (Ruidas et al. 2023). High E.C. values can signify salinity, contamination, or other adverse conditions. pH is the least significant feature for predicting Class 0, having a relatively minor impact. Groundwater samples with high E.C. values (> 1.26) are likely to be classified as Class 0 (poor quality). Conversely, low EC values and pH levels within a certain range contribute less to negative class predictions (Singha et al. 2021).

For positive class predictions (Class 1), another bar graph in Fig. 13 represents the contribution of different features. SAR is a significant feature for predicting Class 1 (favorable groundwater quality). Low SAR values indicate better water quality for irrigation, while high SAR values can lead to soil degradation due to sodium accumulation. TDS is also influential, with low TDS values, desirable for irrigation water. High TDS levels can negatively affect soil structure and plant health. E.C. is important for predicting positive groundwater conditions, with optimal EC values ensuring efficient nutrient transport to plants. Extremely high EC may indicate salinity issues. Groundwater samples with low SAR, low TDS, and moderate E.C. are likely to be classified as Class 1 (good quality), which is favorable for irrigation and sustainable agriculture (Trabelsi and Bel Hadj Ali 2022). XGBoost provides valuable insights for informed decision-making in groundwater management, taking into account both positive and negative quality aspects (Roy et al. 2023).

Inverse distance weighting

Inverse distance weighting (IDW) is a widely utilized spatial interpolation technique that predicts values for a grid by combining the known data points, with weights inversely related to the distance from those points. The premise is that closer points have a greater impact on the estimated value, making IDW particularly effective when the available data is sparse and unevenly distributed (Arkoc 2022; Bordbar et al. 2023); ; .

The IDW interpolation formula is expressed as follows:

$$z(x) = \frac{{}_{i=1}^{n} w_i z_i}{{}_{i=1}^{n} w_i}. \tag{16}$$

In Eq. 16,

- $z(x)$ represents the interpolated value at a given location x,
- z_i denotes the observed value at the ith location,
- w_i signifies the weight corresponding to z_i, and
- n refers to the total number of sample points (Raheja et al. 2022). The weight w_i is calculated as:

$$w_i = \frac{1}{d_i^p} \tag{17}$$

where d_i is the distance from x to i, and p is the power parameter. The power parameter regulates the rate at which the weights diminish with distance; higher values result in steeper weight decay and more localized interpolation.

The groundwater quality prediction utilizing the IDW approach is demonstrated by the IDW interpolation graph in Fig. 14 (Singh and Verma 2019). The x- and y-axes of the graph, respectively, show the Easting and Northing coordinates (Jiang et al. 2022). This representation shows various categories of groundwater quality, where marginal regions are shown in yellow, safe places are indicated by green colors, and red demonstrates hazardous zones. In other words, IDW interpolation is used mostly to predict groundwater quality when scanty and spatially distributed data are in irrigated areas. It is based on the concept that values from unsampled points will bear a closer resemblance to those from adjacent sampled locations. This approach works especially well, in situations, when surface values must be constant, but there is doubt about the precision or possible inaccuracies in the sampled data (Mallick et al. 2022).

The spatial distribution of groundwater quality across the study highlights the influence of both natural and anthropogenic factors in driving its degradation. Geogenic processes such as evaporation, ion exchange and minerals dissolution, contribute to elevated electrical conductivity and salinity in arid and semi-arid regions (Li et al. 2013). At the same time, intensive agriculture activities including excessive use of pesticides, fertilizers and poor irrigation practices has accelerated the leaching of nitrates and other pollutants into aquifers leading to further deterioration (Qureshi et al. 2021). Overextraction of groundwater for irrigation also plays a critical role, lowering water tables and increasing the concentration of dissolved salts through evapoconcentration processes (Gaagai et al. 2023). These combined pressures explain the observed variability in groundwater suitability for irrigation, as detected by IDW interpolation.

Model validation and performance evaluation

The GB model was validated using the 2019 dataset obtained from SCARP Monitoring Organization (SMO) and the 2025 dataset collected from Soil and Water Testing Laboratory, Rahim Yar Khan. The GB model validation results shows excellent predictive accuracy, with RMSE = 0.00, MSE = 0.00, and R = 1.00 for both 2019 and 2025 datasets. Figure 15 illustrates the temporal variation in water quality from 2019 to 2025. The heatmap demonstrates discernible temporal shifts, showing gradual decline in hazardous water sites and a relative improvement in safe water zones, thereby confirming the model's ability to capture both historical and future changes in ground water quality with high reliability (Raheja et al. 2024).

Recommendation for irrigation water quality management

Based on the spatial analysis of groundwater quality using IDW interpolation, it is recommended that irrigation water quality in Rahim Yar Khan needs to be actively managed to prevent further deterioration. Areas identified as hazardous should be promoted to have controlled irrigation practices

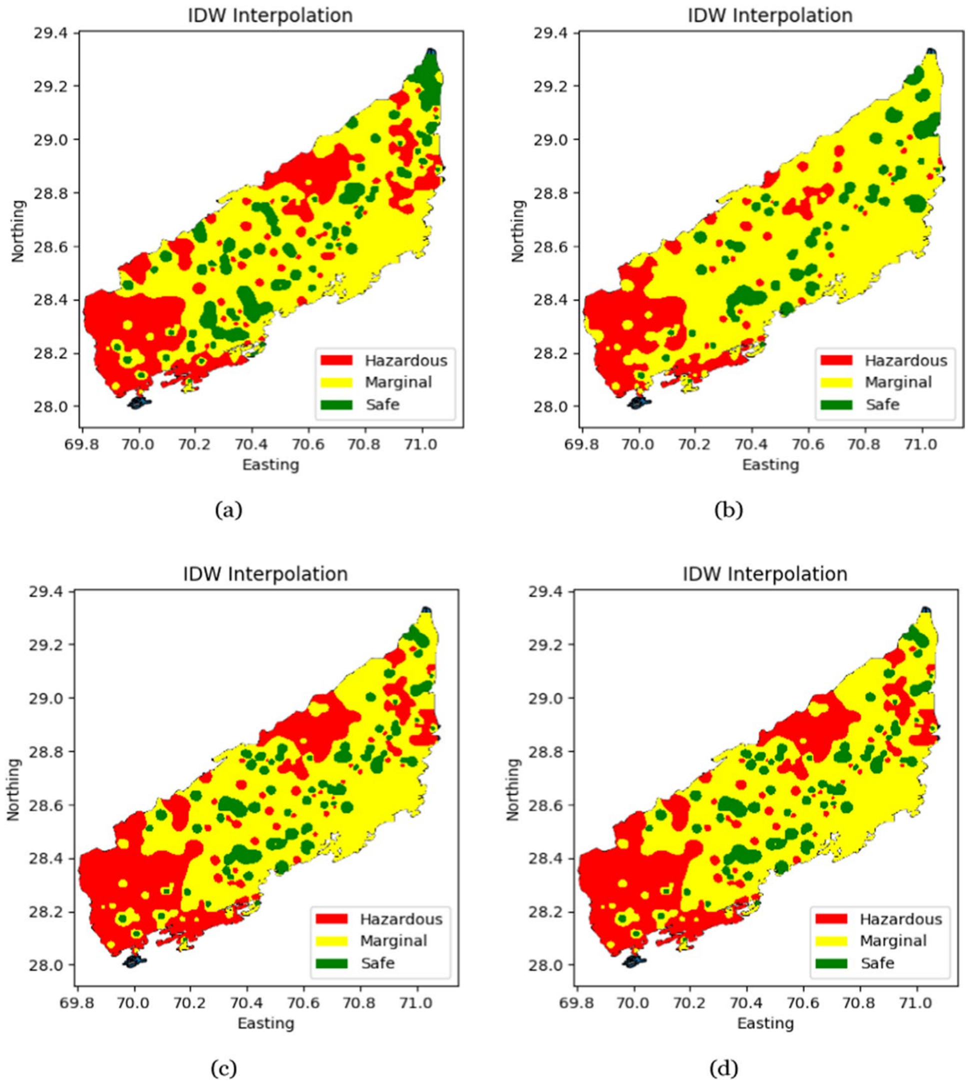


Fig. 14 IDW Interpolation for **A** RF, **B** LR, **C** SVC, **D** GB Model

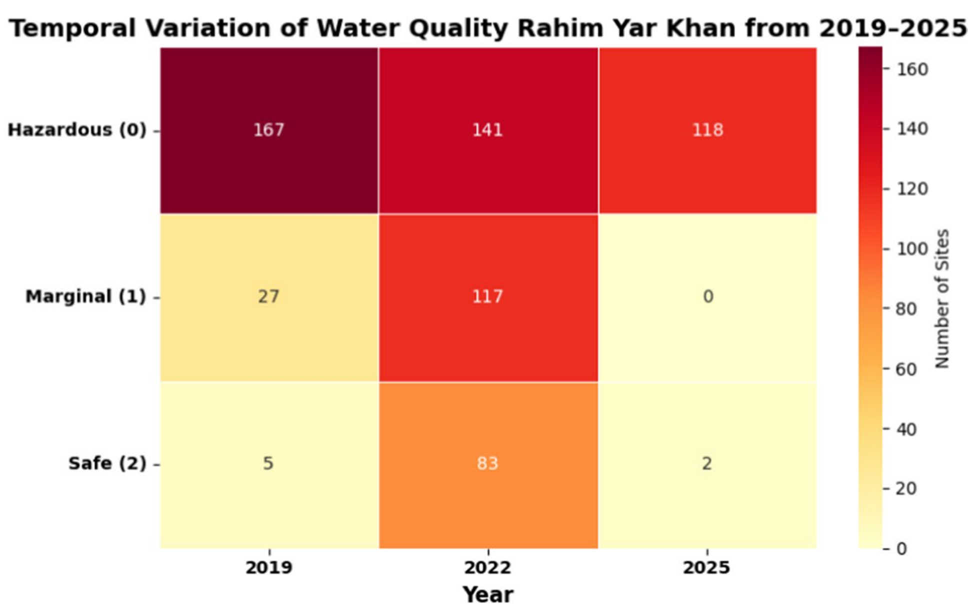


Fig. 15 Temporal variation of water quality Rahim Yar khan from 2019–2025

and low delta crops to limit excessive water withdrawal and reduce stress on aquifers. Promotion of artificial intelligence practices such as recharge wells can enhance replenishment of clean water into aquifers. Regular monitoring of groundwater quality is essential to detect early signs of contamination and implement adaptive management strategies. Additionally, awareness programs for local framers on sustainable irrigation practices can help reduce anthropogenic impact on groundwater resources.

Conclusion and future work

This research employed an ensemble-boosting Gradient Boosting (GB) model to evaluate the groundwater quality in the Rahim Yar Khan irrigation system in Pakistan. Groundwater quality management in this region is currently inadequate. Implementing machine learning techniques for this purpose could significantly lower the costs associated with for groundwater quality testing. Various machine learning models were employed for performance comparison as well. Feature engineering methods are utilized to identify essential water quality indicators before integrating them into machine learning models. A color-coded map is used in the study to illustrate different groundwater quality zones: yellow for marginal quality, green for safe water, and red for hazardous water. The study findings reveal that groundwater distribution consisted of 17.34% hazardous areas, 79.36% marginal areas, and 3.30% safe areas, which is determined using the inverse distance weighting interpolation technique. The GB model demonstrated an effective performance by accurately predicting the groundwater quality index with a 99% accuracy. Furthermore, it effectively reduced the number of required parameters while preserving the model's accuracy. By eliminating redundant and inconsistent data, the approach improved both model accuracy and training speed. Economically, it saves time and costs related to measuring water quality parameters and helps prevent inaccuracies resulting from manual measurements, leading to reliable groundwater quality assessments. By implementing machine learning methods, we can overcome several limitations of traditional approaches. Thus, this study offers a promising alternative for predicting groundwater quality in irrigation systems and similar environments, with a minimal set of parameters. Future research will focus on exploring advanced machine learning models or deep learning models to further increase the performance of groundwater quality index calculations.

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Data availability Data is available from the authors upon reasonable request.

Declarations

Conflict of interest The authors declare that there is no conflict of interest regarding the publication of this paper.

Ethical statement Not applicable.

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