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Predictive Modeling and Risk Assessment of Groundwater Quality Using Machine Learning Techniques: A Case Study of India

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Predictive Modeling and Risk Assessment of Groundwater Quality Using Machine Learning Techniques: A Case Study of India

by

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Abstract

The quality of groundwater is a matter of high concern in India, as millions depend on it for drinking water, agriculture, and industry. In this context, the present study makes an attempt using machine learning models to predict and classify the quality of groundwater with respect to essential water quality parameters, namely pH, temperature, and conductivity. This paper therefore introduces a predictive framework based on the higher-order machine learning techniques of XGBoost, Random Forest, Support Vector Machine, and Logistic Regression to assess the quality of groundwater across several regions in India. Among these, the most precise-one with 97.13% accuracy-was from XGBoost, followed by the Random Forest, which had an accuracy of 96.36%.

A novel WQI-based risk-scoring algorithm was also developed, classifying water quality between "Excellent" and "Poor." The proactive approach developed for policymakers and environmental agencies basically empowers early intervention in regions prone to groundwater contamination, especially due to fluoride and industrial pollutants.

Here, the machine learning models outperform conventional methods of groundwater assessment using large datasets and tracking subtle contamination patterns. The integration of machine learning into comprehensive water quality datasets expands the predictive capability of the models for compatibility with real-time monitoring and scalability across various regions. Though the model efficiencies were found to be high, this study recognises some of the limitations, including data imbalance and lack of temporal trends within the data. Future research should, therefore, consider expanding the dataset to a wider geographical scope and, where possible, include time-series data to aid in the prediction of long-term trends in groundwater quality. The present research provides a sound basis for data-driven groundwater management in view of the ever-increasing demands on sustainable water supplies.

ACKNOWLEDGEMENTS

I would especially like to thank Dr. Jing Wang for agreeing to be my supervisor and for his consistent advice, feedback, guidance and support throughout the lifecycle of this ‘Predictive Modeling and Risk Assessment of Groundwater Quality Using Machine Learning Techniques: A Case Study of India’ project.

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1. INTRODUCTION

1.1 Background and Context

- **Importance of Groundwater Quality:** Groundwater represents a very vital resource, which caters to the needs of more than two billion people around the world in the form of drinking water, water for agriculture, and water for industries. In some countries like India, it is the major source of freshwater to big sections of the population, particularly in rural areas. With the increasing demand for clean water, the quality of groundwater becomes an important factor for public health, agriculture, and further sustainable development. Contaminated groundwater may lead to serious health problems, environmental deterioration, and economic loss. Therefore, the quality of this resource should be monitored and maintained at all costs.
- **Management of Groundwater Quality:** Challenges - There are risks to groundwater from natural and anthropogenic sources of contamination. Groundwater may get infiltrated by contaminants like heavy metals, industrial waste, pesticides, and fluoride, making them unusable. Traditional methods of assessment of groundwater quality have been usually based on physical collection of samples and subsequent laboratory analysis-a time-consuming process with limited scope. Besides, these methods are often not effective to identify patterns of contamination over large geographical areas or in predicting future changes in water quality.
- **Overview of Machine Learning in Environmental Science:** It goes on to promise that machine learning answers the question through the facilitation of pattern identification and making of predictions upon large datasets analysis. ML algorithms can process, therefore, a very complex and multi-dimensional data with the ability to come up with correlations between the various water quality parameters that would have otherwise not been realized. In environmental science, ML has found broad applications such as climate prediction, habitat mapping, and classification of groundwater quality. Through the application of ML, researchers create predictive models to classify groundwater quality, determine the risks of contamination, and help drive decisions toward sustainable water management.

1.2 Problem Statement

- **Short Comings in the Present Assessment of Groundwater Quality:** Most traditional methods of monitoring groundwater are incapable of detecting wide-scale contamination or issuing early warnings on quality degradation. Essentially, they are reactive rather than proactive, with limited insight into the trend of emerging contaminations. Apart from that, most of these methods concern local areas and cannot be upscaled to regional or national levels. Not being able to predict the future groundwater conditions based on historical data is considered a major gap in the existing approaches to groundwater quality management.
- **Predictive Models:** New demands are arising for advanced machinery capable of not only assessing present conditions but also foreseeing future risks regarding groundwater pollution. Such challenges can be answered by machine learning models combined with extensive data on any given area and time, predicting the quality of groundwater quite accurately. By applying such predictive models, governments, agencies, and communities will be in better positions to deal more effectively with the management of groundwater resources through timely interventions in areas highlighted as high risk.

1.3 Objectives

- **Main Objective:** To develop a machine learning-based framework for the classification of groundwater quality and risk area prediction, including the development of a strong model which will use key water quality parameters like pH, temperature, and conductivity that can accurately identify the quality of the groundwater.
- **Specific Objectives:**
  - **Classification of Ground Water Quality:** Use the water quality dataset to develop machine learning models to classify ground water into "Excellent," "Good," "Moderate," or "Poor." Based on the WQI, develop a risk scoring algorithm so as to recognize the high-risk areas with regard to contamination by fluoride, industrial pollutants, etc.
  - **Actionable Insights:** Integrate machine learning predictions with geographical data to provide real value for the decision-makers through targeted interventions in groundwater management.
  - **Scalable and Replicable Model:** The models developed should be scalable and replicable on different regions and different datasets to extend applicability for a wide range of environments in groundwater quality management.

2. Literature Review

2.1 Introduction

Groundwater is among the most highly valued natural resources on Earth and plays a core role in supporting ecosystems and human activities. This resource constitutes a major source of water supply for drinking, agriculture, and industry in many parts of the world. According to Simlandy (2015), groundwater is highly valuable due to its availability and diverse applications, such as household consumption, irrigation, and industrial processes. Despite its abundant supply, the quality of groundwater is frequently overlooked, which can lead to serious ecological and societal problems if left unchecked (Simlandy, 2015).

Groundwater is a renewable resource; it is replenished on an annual basis by rainfall. However, through both natural processes and human activities, its quality will gradually deteriorate. While passing through the soil and rock formations, the moving groundwater can dissolve contaminants like heavy metals, pesticides, and chemicals, thus making it unfit for consumption (Smedley & Kinniburgh, 2002). This project deals with predictive modelling for classifying India’s groundwater quality employing machine learning techniques. The models give useful information on risks that can result in the contamination of water and further help in elaboration for plans on sustainable management.

2.2 Machine Learning in Environmental Science

Machine learning has revolutionized environmental science to develop capabilities in processing voluminous, complicated datasets that other traditional statistical methods cannot venture to provide meaningful interpretation. According to Zhong et al. (2021), the flexibility of machine learning lies in its ability to handle multidimensional data and uncover hidden patterns, making it ideal for applications in environmental monitoring and risk assessment. Moreover, ML allows for the development of predictive models that can estimate future trends in groundwater contamination based on historical and real-time data (Zhong et al., 2021).

Groundwater quality classification modeling has attracted considerable interest due to its potential integration with various influencing factors like chemical composition, geology, and climate. This provides an important tool for developing predictive modeling that may identify contamination so that suitable strategies can be pursued for sustainable management. For example, predictive models have been applied to monitor arsenic levels in groundwater, providing more accurate and timely warnings for affected areas (Zhong et al., 2021). By using machine learning techniques, environmental scientists can now build more efficient systems to protect vital water resources and mitigate the risks associated with groundwater contamination.

2.3 Existing Research on Groundwater Quality Classification

2.3.1 Study 1: Arsenic Contamination in Groundwater of West Bengal (Chakraborti et al., 2002)

This study by Chakraborti et al. (2017) concerned arsenic contamination in groundwater throughout West Bengal, India. Various water samples were analyzed for their concentration of arsenic and were correlated with health effects like skin lesions and cancer cases among the residents. No machine learning model, such as decision trees or neural networks was implemented; traditional statistics were used to create a map and predict the contamination risk.

Key Findings:

- By using statistical methods to analyze the data, the study effectively highlighted the scope and severity of the arsenic problem. The correlation between groundwater arsenic levels and health impacts helped to reinforce the need for policy changes and increased awareness among the local population.
- The statistical analysis showed that approximately **48%** of samples had arsenic levels greater than 10 µg/L, and **23.8%** had levels higher than 50 µg/L. This highlighted a significant proportion of the population at risk.
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2.3.2 Study 2: Groundwater Quality Assessment Using GIS and Remote Sensing (Asadi et al., 2007)

This study applied GIS and remote sensing to the assessment of groundwater quality of Hyderabad. The study mapped the spatial distribution of pollutants such as Total Dissolved Solids (TDS), nitrates, and fluorides. The WQI was computed in order to judge the suitability of groundwater for drinking purposes. Most of the study relied on spatial mapping and did not incorporate predictive models for the future quality of groundwater.

Key Findings:

- Spatial analysis revealed that areas like Erragadda had TDS levels as high as 1350 mg/L, indicating significant contamination.
- Water Quality Index (WQI) indicated that many areas had poor water quality, unfit for drinking purposes.

2.3.3 Study 3: Water Quality Assessment and Modelling Using Machine Learning (Mishra et al., 2020)

The models of machine learning, including ARIMA, used in this study, draw inferences on the assessment of the groundwater quality in the Ayodhya district of Uttar Pradesh. The data from 97 samples of groundwater collected during the period from 2000 to 2018 were utilized for the prediction of the WQI and water quality classification. By including the seven hydro-chemical parameters, namely pH, calcium, magnesium, chloride, sulphate, nitrate, and fluoride, into the model, one can predict the quality of the groundwater. The ARIMA model predicted successfully the future values of WQI that could identify the area at risk due to contamination.

Key Findings:

- The ARIMA model provided accurate predictions of Water Quality Index based on historical data, allowing for early detection of contamination risks.
- The machine learning approach showed better accuracy compared to traditional manual calculations.

2.4 Gaps and Limitations in the Existing Research

1. **Limited Applications of Predictive Models for the Groundwater Quality:** While some studies, such as Mishra et al. (2020), adopt machine learning techniques, so far the overwhelming majority of works rely on traditional methods (Chakraborti et al., 2002; Asadi et al., 2007). No comparative analysis between different machine learning models can be found for the quality of groundwater.
2. **Geographic Scope:** The existing literature is confined to specific regions, such as West Bengal or Hyderabad. Replication in other regions of India may therefore yield very different findings due to differing geological and environmental settings.
3. **Temporal Predictions:** Works such as Asadi et al. (2007) consider only the spatial distribution and give no indication of changes in time or risk in the future. In fact, these could be predicted using various machine learning models, for example ARIMA or LSTM.

2.5 Justification for Current Research

The proposed research will fill the knowledge gaps in the literature by applying machine learning models for the prediction of groundwater quality in most regions of India. This will enhance the predictability and generalizability of the models that shall be useful for decision-makers and environmental agencies to frame and implement proper policies regarding groundwater management. Advanced machine learning techniques, such as neural networks and deep learning, may further improve the accuracy of predictions of groundwater quality to address both spatial and temporal variations.

3. System Analysis

3.1 Legal, Social, Ethical, and Professional Issues

There are several legal, social, ethical, and professional issues with the implementation of machine learning models for prediction in groundwater quality. These issues should be analyzed in detail so that the system will be at full compliance with regulatory frameworks, socially responsible, and protectively professional regarding handling data and the environment.

- **Legal Issues:** The legal issues pertaining to the use of environmental data, especially the groundwater monitoring data, are very important. Access to public water data from government agencies, such as CPCB, should be conditioned on the regulation concerning data use and dissemination. Other concerns arise when the data involves location-based groundwater, or private lands are involved, and the release of certain water quality data may affect property value or even lead to court battles. Moreover, there is a need for observance of regulations on the use of predictive models in environmental management to ensure outputs from the machine learning models are not used for purposes other than those serving the public interest.
- **Social Issues:** Groundwater quality has major social concerns, primarily impacting areas where access to clean water is at a premium. The application of machine learning models in the prediction of water contamination empowers the community through early warnings on deteriorating water quality. On the other end, this might pose a risk of creating fear or distrust in a particular area once water quality issues are revealed without ways of mitigation. Secondly, the system has to consider inequities in the socio-economic setting of access to water infrastructure and resources by ensuring that the benefits of such a system are equitably shared, not

making communities that are more vulnerable bear a disproportionate impact of water quality.

- **Ethical Issues:** Some of the ethical issues involved in the development of this system surround data ethics, transparency, and accountability. These machine learning models require large datasets to be trained on, and every precaution must be taken to ensure that such data is sourced in an ethical manner, considering its utilization so as not to allow the occurrence of bias in predictions, which could mean misrepresenting certain regions. Also, clarity needs to be shed on the decision-making process for the models so that "black box" predictions will be evaded-neither the stakeholders nor users being able to make sense or believe them. The system must prioritize affected population wellbeing, guarantee that predictions are employed to benefit public health and prevent further harm. Whereas ethical issues could arise if it is for commercial purposes-land development or privatization of water resources among others, the model shall predict.
- **Professional Issues:** The system should be developed on professional grounds by the engineers and data scientists. In particular, accuracy, reliability, and integrity of the design and deployment of the models should be guaranteed. For this system, rigorous testing and validation should be performed by the professionals in charge to ensure that the models yield reliable and accurate results since environmental and public health implications are very related to it. Also, experts should explain succinctly what the models cannot do so that stakeholders are aware of the context and uncertainties that might arise associated with machine learning predictions in environmental science. Interdisciplinary interactions with relevant environmental scientists, hydrologists, and policy analysts will help ensure the system's relevance and effectiveness in real-world applications.

4. METHODOLOGY

4.1Research Design

4.1.1 Explanation of chosen research design:

The proposed research design is an experimental approach that applies machine learning algorithms to classify the quality of groundwater by setting a set of features. These include data collection and pre-processing followed by model selection of the different machine learning algorithms. Accordingly, the proposal intends to develop predictive models for the evaluation of groundwaters quality with insight into risks factors that may affect the safety of the water. This involves data cleaning, feature engineering, and evaluation of the model to ensure that the selected models generalize efficiently on unseen data.

4.2 Machine Learning Models

4.2.1 Selection Criteria for Models:

The nature of the dataset, problem type (classification) and interpretability criteria are the main factors for machine learning model selection. Preference was given to models that were renowned for their high accuracy, robustness toward overfitting, and interpretability. In selecting the models, the following were considered:

- Accuracy of Model Performance in related tasks of classification
- Ability in handling imbalanced datasets
- Interpretability of results
- Computational efficiency and scalability

4.2.2 Description of Models Used:

1. **Logistic Regression:** Simple but efficient linear model for binary classification; it estimates the probability of a given input belonging to a particular class.
2. **Random Forest**: One of the versatile ensemble methods, constructing several decision trees and combining the predictions; it is robust against overfitting and copes well with nonlinear relationships.
3. **Support Vector Machine (SVM):** One of the powerful classification models which works quite well with high-dimensional data. Find a hyperplane that can do an excellent job in the separation between classes.
4. **XGBoost:** It is one of the advanced gradient-boosting algorithms for the purpose of classification. It is also rather versatile and capable of capturing very complex data.

4.3 Risk Scoring Framework

4.3.1 Development of the Risk Scoring Model:

The framework for risk scoring in this project is developed using the Water Quality Index (WQI) metric. Generally, an index is used to represent comprehensive data with just one number, reflecting the quality rating at any given location for water quality. In this study, three important water quality parameters have been considered as the WQI: pH, temperature, and conductivity. Each parameter adds up the final WQI according to its influence on the water quality, and the integrated score is used to evaluate the integrated risk linked with the groundwater.

4.3.2 Risk Scoring Metrics and Criteria:

Following are the metrics and criteria that have been used to score and classify the water quality:

- **Water Quality Index (WQI):** It is a single value for the aggregate water quality, in which a higher WQI score means poorer water quality.
- **Model Calibration:** Class-wise calibration curves are created in order to understand the accuracy of the probabilities predicted for each water quality class: "Excellent", "Good", "Moderate", and "Poor". The class-wise calibration shows where the model has cases of being under-confident or overconfident in predictions, particularly around the critical probability thresholds of decisions.

4.3.3 Class-wise Analysis

- **Excellent Class**: Indeed, the model does show divergence from the ideal calibration line at low and high predicted probabilities, possibly suggesting under-confidence and overconfidence with their misclassification risks. (WQI <= 25)
- **Good Class:** The calibration of the model for this class is really far from ideal, which would mean poor reliability in at least the range of probabilities between 0.3 and 0.7 for the model's predictions. (25 < WQI <= 50)
- **Moderate Class:** There are significant oscillations within the calibration curve, reflecting under-confidence for low probabilities and overconfidence at higher probabilities. (50 < WQI <= 75)
- **Poor Class:** Fairly good calibration of the model for high probabilities; the model tends to be underconfident for mid- to low-probability situations. (WQI > 75)

This risk-scoring framework identifies high-risk water quality zones by combining the WQI and model calibration results. The predictions obtained from this model, along with their confidence, minimize the risk of misclassification-that is, predicting "Moderate" or "Poor" water quality incorrectly.

4.4 Validation and Testing

4.4.1 Methods for Validating the Accuracy and Effectiveness of the Models:

The validation of the models used for groundwater quality classification was performed using several methods to ensure the accuracy, robustness, and generalization ability of the predictions. These methods include:

- **K-Fold Cross-Validation**:
  - The data is divided into k number of subsets or folds where each fold acts as a validation set and remaining folds act as a training set. This process gets repeated k number of times, normally 5 or 10 with the aim of ensuring that every observation has appeared in both training and validation.
  - This method helps prevent overfitting and ensures that the model performs consistently across different data splits.
- **Hold-Out Validation**:
  - Typically, it considers holding out 20-30% of the data for testing and uses the rest for training. Once the model is fitted, its performance on hold-out test data gives a reasonable estimate of the model's performance when applied to unseen data.
- **Confusion Matrix**:
  - The confusion matrix will plot and assess the performance of the models by matching predicted classes to real ones. Metrics such as true positives, false positives, true negatives, and false negatives are used in the derivation of key performance indicators such as precision, recall, and F1-score.
- **Calibration Curves**:
  - Calibration curves plot the predicted probabilities against the observed outcomes in order to establish the capability of the model in predicting exact probabilities. This would be perfectly calibrated if the perfect correspondence between predicted probability and the observed outcome is attained. In water classification problems, this technique could be very useful in determining the risk of misclassification.

4.4.2 Testing Procedures:

1. **Performance Metrics**: The models are evaluated based on several key metrics to measure their classification performance:

- **Accuracy**: Measures the percentage of correct predictions across all classes.
- **Precision**: Evaluates how many of the predicted positive cases (e.g., "Poor" water quality) were actually correct.
- **Recall (Sensitivity)**: Measures the model's ability to identify actual positive cases (e.g., identifying all instances of "Poor" water quality).
- **F1-Score**: The harmonic mean of precision and recall, providing a balanced evaluation when dealing with imbalanced datasets.
- **Area Under the ROC Curve (AUC-ROC)**: Used to assess the trade-off between sensitivity and specificity, particularly for high-risk water quality classifications.

2. **Error Analysis**:
   - Misclassifications and borderline cases are mainly reviewed in search of a pattern or source of error when the model has low confidence. Special attention is taken with the "Moderate" and "Poor" classes since there could be more overlap in their respective feature spaces, which leads to a higher possibility of misclassifications. Final Model Selection

3. **Final Model Selection**:

   - The models are ranked based on their performance across all evaluation metrics. The model that demonstrates the best balance of precision, recall, and F1-score, while also showing good calibration, is selected as the final model for predicting groundwater quality. Special consideration is given to its performance on high-risk categories (e.g., "Poor" water quality).

4.4.3 Testing Pipeline:

1. **Data Preprocessing**: Ensure that the test data undergoes the same preprocessing steps (e.g., imputation of missing values, feature scaling) as the training data.

2. **Model Application**: Apply the trained model to the test set.

3. **Prediction Interpretation**: Generate predictions and probabilities for each sample.

4. **Performance Evaluation**: Compare predictions against the actual labels and compute evaluation metrics.

5. **Calibration and Risk Adjustment**: Adjust thresholds and calibrate probabilities for final risk scoring.

This comprehensive validation and testing process ensures that the models not only perform well on the training data but also generalize effectively to new, unseen data while providing reliable risk scores for groundwater quality.

5. Data Overview

5.1 Data Sources

The principal dataset used in the following analysis was sourced from the official website of the Central Pollution Control Board, Government of India, under the source of the National Water Monitoring Programme. This includes the data for the quality of groundwater across various stations in India from 2012 to 2021 and each dataset is collected and combined as a single CSV file "GROUND.csv."

Source: Central Pollution Control Board (CPCB). National Water Monitoring Programme (NWMP) Groundwater Data. Retrieved from https://cpcb.nic.in/nwmp-data/.

The secondary dataset "states_India.geojson", which was used for geospatial visualization, was obtained from a tutorial on GitHub source. The Choropleth maps of the spatial distribution of water quality over Indian states will be plotted by taking the necessary input from this file.

Source: Nikhil Kumar Singh. GeoJSON file for Indian States Choropleth Maps. GitHub Repository. Retrieved from https://github.com/nikhilkumarsingh/choropleth-python-tutorial/blob/master/states_india.geojson.

5.1.1 Justification for Choice of Data Source:

Comprehensive data: Water quality dataset is pretty comprehensive, ranging over several years, with a set of crucial parameters like pH, Temperature, Conductivity, among others, really important to describe the quality of groundwater.

Reliable and official: The data is published by a government body, hence credible and relevant to environmental research.

Geo-spatial Analysis: A geojson file showcasing the boundaries of the states to effectively portray the geography to enhance regional variation in water quality.

5.2 Dataset Characteristics

The dataset contains 7872 entries with 10 attributes representing the groundwater monitoring across multiple stations in India. The key characteristics of the dataset are presented below:

- **Station Code:** The unique code assigned for every monitoring station.

- **Station Name:** The name of the specific monitoring station.
- **State:** Indian State where the station falls.
- **Temperature (Min and Max):** Minimum and maximum water temperatures recorded at the observation sites.
- **pH (Min and Max):** Levels of groundwater acid or alkaline.
- **Conductivity (µmhos/cm) Min and Max:** The conductivity is a reflection of the ionic content of the water.
- **Year:** Year in which the data was collected, ranging from the year 2012 to 2021.

Statistical Overview:

- **pH values**: Range from 0 to 9.6, with a mean of approximately 7.1.
- **Temperature values**: The minimum recorded is 0°C, and the maximum is 70°C, with an average of 25.3°C.
- **Conductivity**: Varies widely, from 0 to 87,790 µmhos/cm, indicating significant regional differences in water quality.
- **Years**: The data spans from 2012 to 2021, with more entries concentrated in recent years.

5.3 Data Preprocessing

Preprocessing was necessary to make the dataset sufficient for machine learning. The handling of missing values, cleaning inconsistencies, and preparation of different columns are discussed here in several steps.

5.3.1 Steps Taken for Cleaning and Preprocessing Data:

1. **Missing Values Analysis:**
    - The initial check showed that important columns like **Temperature, pH, and Conductivity** have many missing values. The total number of rows originally present was **7872**; after the cleaning of missing data, it was reduced to **7043.**
    - **Station Code:** Some missing values were found, but since this was not important for the modeling aspect, it was left with missing entries.
    - **STATE:** The rows containing the missing state names were removed because doing an analysis at the state level, without it, is important and can't be done in this case.
    - **Critical Parameters** (pH, Temperature, Conductivity): Missing values have been imputed taking into consideration of State and Year by a context-sensitive method.
2. **Missing Value Imputation:**

- **Median Imputation:** Numerical columns such as Temperature Min, pH Min, Conductivity Min have been imputed using the median instead of the mean since the median is generally more resistant to outliers
- **Contextual Imputation:** Instead of applying a global median across the entire dataset, the data was grouped by **State** and **Year**, and the median was calculated within each group to account for the regional and temporal differences in water quality.
- After applying this method, the missing values for these columns were filled in, resulting in a more complete dataset with **0 missing values** in key columns such as **pH** and **Conductivity**.

3. **Outlier Detection:**

- The Conductivity and pH columns reported outliers; some of the values in these columns were rather extreme and were detected as errors. For instance, a **pH** of 0 or a **Conductivity** of **87,790 µmhos/cm** were then changed using domain knowledge or removed so that these would not distort the training process of machine learning models.
- In the case of pH, the range was trimmed to a more reasonable range, considering it should be within 6 to 9. Regarding conductivity, the values were capped to known environmental limits.

5.3.2 Missing or Inconsistent Data Handling:

- **Consistency in State Level:** There were some inconsistencies in the spelling/misaligned entries of the state names. These were standardized for uniformity and to ensure successful merging of the geospatial data for visualization.
- **Station-level:** There were cases found with misaligned station codes or duplicated entries. These were checked laboriously, and the most reliable entries were kept after removing the duplicates.

5.3.3 Cleaning Process Overview:

- The raw dataset contained **7872 rows** and 10 columns, and after cleaning, by deleting rows due to missing and inconsistent data, the preprocessed data contained **7043 rows** and 9 columns.
- The **Station Code**, which had blank entries, was not important for the machine learning models; thus, it was retained as such.

- Important features in Temperature, pH, and Conductivity were cleaned and imputed, after which there were no missing values left in the dataset.

This comprehensive cleaning and preprocessing step prepared the data into a harmonious, no-missing value, and feature engineering-ready state for model development.

5.4 Data Transformation

5.4.1 Techniques Used:

Below are the some of the data transformation techniques employed for this project to ensure that the data was prepared for machine learning algorithms. This consists of normalizing the data, feature engineering, and any other steps necessary to better the model's performance.

1. **Normalization:**
   - **Min-Max Scaling:** Temperature, pH, and conductivity are all continuous features that were normalized by Min-Max scaling to fall under the same range. This ensures that no feature, having a larger numerical range-for example, conductivity-monopolizes the learning process.
2. **Feature Engineering:** Feature engineering was used to extract extra meaningful features from raw data that help the model predict better.
   - One of the important engineering features targeted in this project is the **Water Quality Index (WQI).** It summarizes, in general, the groundwater quality concerning parameters related to pH, temperature, and conductivity. This metric simplifies the classification task because, with the help of the metric alone, it will be able to determine water quality categories such as Excellent, Good, Moderate, and Poor.

   Example: The WQI is computed as a weighted combination of the three main water quality parameters and, hence, provides an idea with respect to the overall quality of the groundwater.

   - **pH and Temperature Average**: In order to iron out the variability in pH and temperature readings, an average was computed for each of these variables. This cleaned the noise in this dataset, enabling the model to learn meaningful patterns instead of huge variations.

5.4.2 Feature Selection:

- **Correlation Analysis:** This was done using a correlation matrix to identify those highly correlated features. Those features identified as being highly affected by multicolinearity were removed or combined to simplify the model without the loss of predictability.

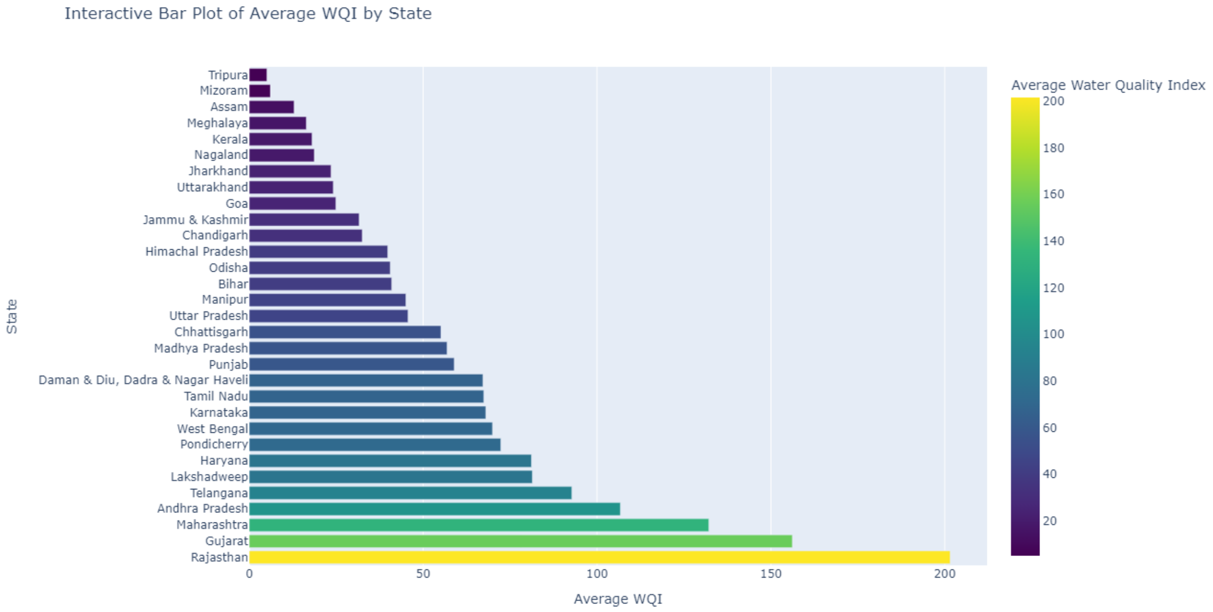
- For instance, **Conductivity Min** and **Conductivity Max** are highly correlated; therefore, taking such features into a mean value instead of independent features will reduce the dimensionality of the feature space.

5.4.3 Data Transformation Statistics:

- **Temperature [Min-Max]:** The temperature ranges between **0°C** and **70°C** and was normalized to be between 0 and 1 to consistently represent across the models.
    - **Mean Temperature:** After normalization, the average temperature of all the stations is about 25° C.
- **pH [Min-Max]:** The pH ranged between 0 to 9.6. Normalizing was the same as in other cases while the average pH across stations is about 7.1.
- **Conductivity:** The range of conductivity goes from 0 to 87,790 µmhos/cm. We normalized the conductivity values in order to have average conductivity across the stations equal to about 1,300 µmhos/cm.

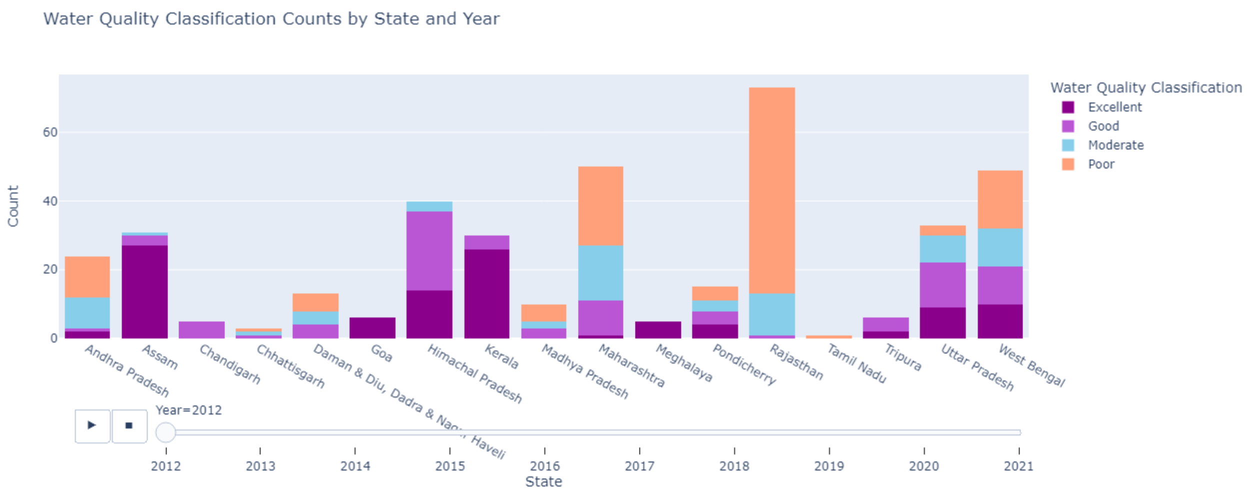
5.4.4 Handling Categorical Data:

- **State Encoding:** The column of "State" contains categorical data. It has one-hot encoding to handle state differences in water quality that machine learning algorithms would take without being biased from the ordinal relationship between states.



5.4.5 Data Transformation to Machine Learning Models:

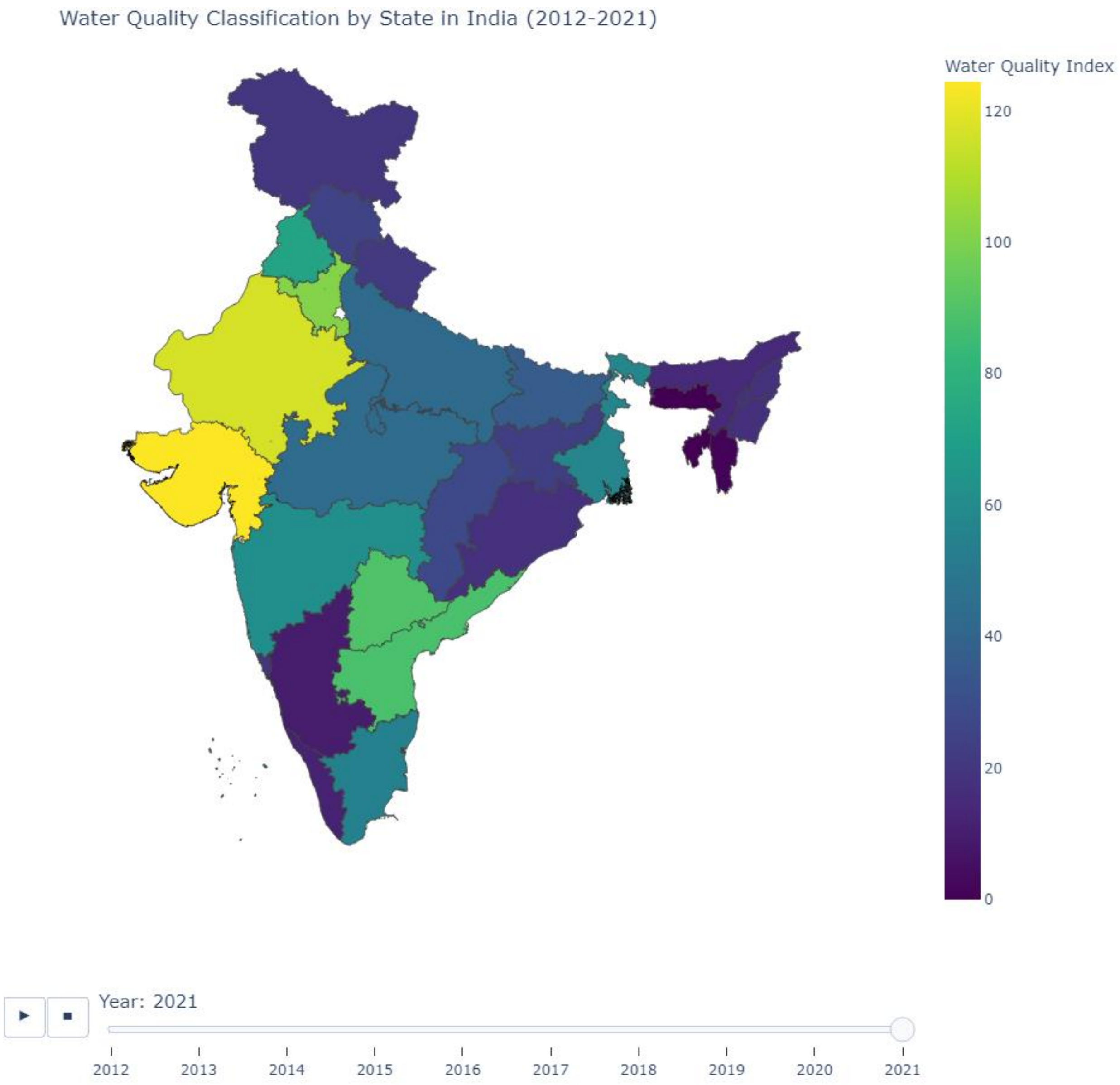
- After all the preprocessing steps and required transformation, the dataset was made ready for machine learning algorithms. It involved the transformation of both input features such as temperature, pH, and conductivity, and the target variable WQI into the format appropriate for a classification model.
    - Further, cleaned and hence transformed data were divided into training and test sets to ensure the cleanness of the data and appropriateness of format for training models.


Water Quality Classification Counts by State and Year

5.4.6 Geospatial Data Integration:

- The **states_India.geojson** file was merged with the water quality dataset based on the state names, enabling geospatial visualizations such as choropleth maps, which help in the geographical analysis of water quality trends across India.

These transformations were some of the most important steps in preparing the data for machine learning, enhancing model accuracy, and improving the interpretability of the results.



6. IMPLEMENTATION

6.1 Model Development

1. **Data Preprocessing:**

- **Feature Scaling (Standard Scaler):**
  - The standardization of features **like Avg Temperature, Avg pH, and Avg Conductivity** ensures that the models (especially those relying on distance metrics, like SVM and Logistic Regression) do not bias predictions towards larger scale features.
- **Formula for Standardization:**

$$z = \frac{x - \mu}{\sigma}$$

where x is the original feature value, μ is the mean, and σ is the standard deviation.

2. **Model Evaluation Metrics:** Each model was evaluated using classification reports which provide detailed metrics like Precision, Recall, F1-score, and Accuracy.

- **Precision:** Measures the proportion of correct positive predictions.

$$\text{Precision} = \frac{\text{True Positives}}{\text{True Positives} + \text{False Positives}}$$

High precision is crucial in this context, particularly for classes like "Poor" water quality, as misclassifying a poor-quality water source as good can have serious environmental and health consequences.

- **Recall (Sensitivity):** Measures the proportion of actual positives that were correctly identified.

$$\text{Recall} = \frac{\text{True Positives}}{\text{True Positives} + \text{False Negatives}}$$

Recall is critical when identifying poor-quality water sources since missing these cases can lead to underestimating risks.

- **F1-score:** The harmonic mean of precision and recall, balancing the two.

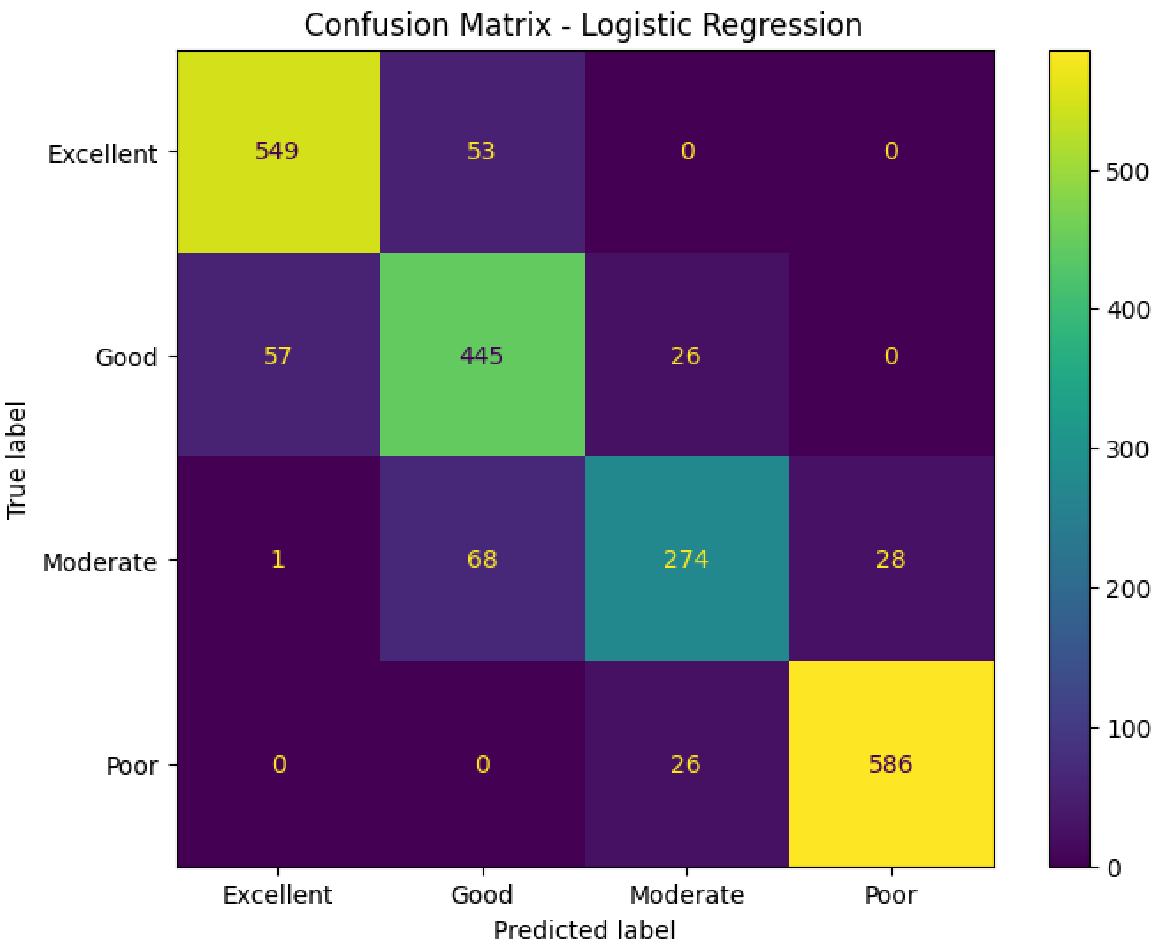
$$\text{F1} = 2 \times \frac{\text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}$$

F1-score is useful when the balance between precision and recall is required, especially for the "Moderate" and "Poor" water quality classes.

3. **Model-Specific Statistical Information:**

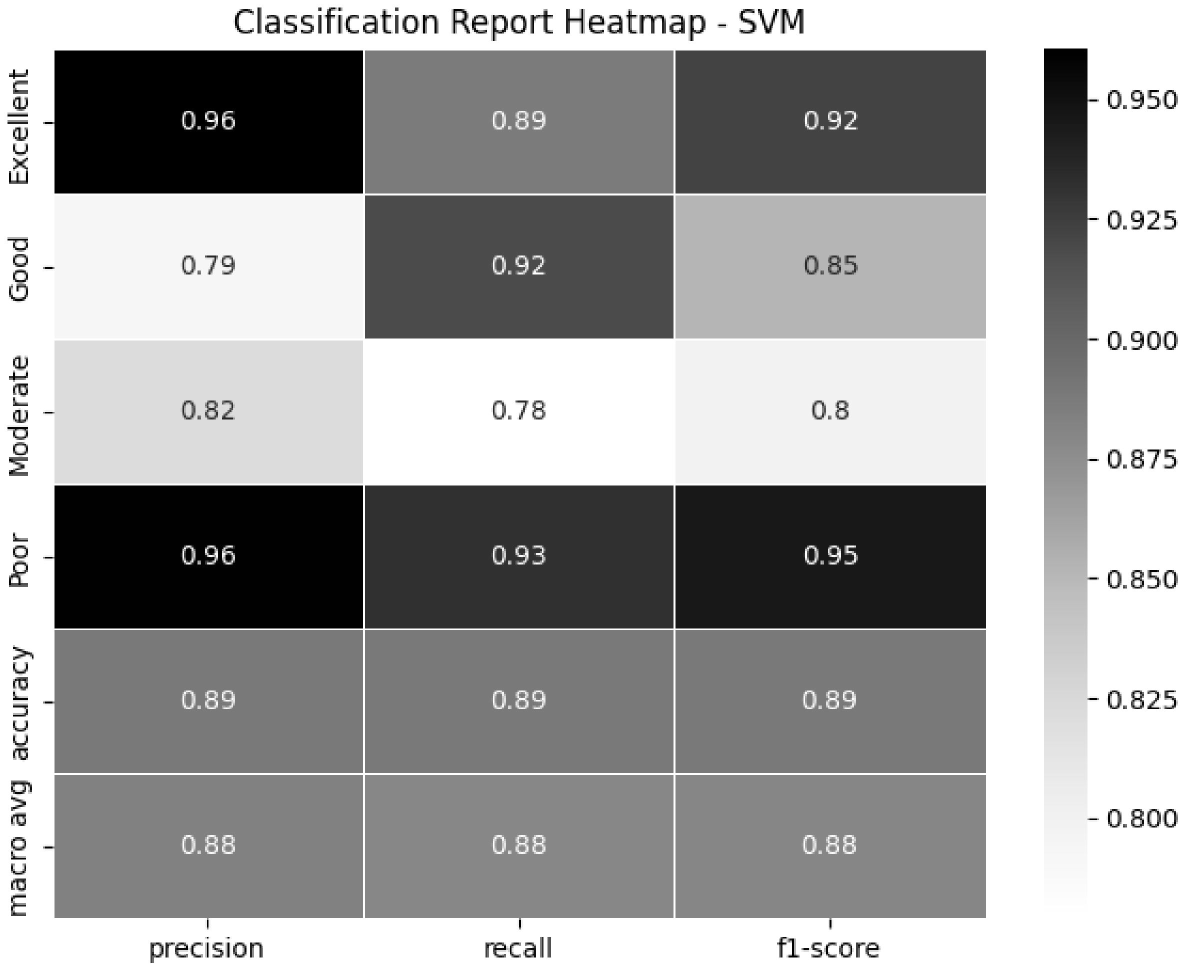
Logistic Regression:

- **Statistical Assumption:** Logistic regression assumes that the log-odds of the target variable (i.e., the probability of being in one of the water quality classes) are linearly related to the feature variables.
- **Coefficients:** The logistic regression model provides coefficients (weights) for each feature that indicate the log-odds of belonging to a class. This can be interpreted as the effect size of each predictor variable on water quality classification.
- **Accuracy:** 87.7% on test data, with a focus on high recall for poor water quality predictions.



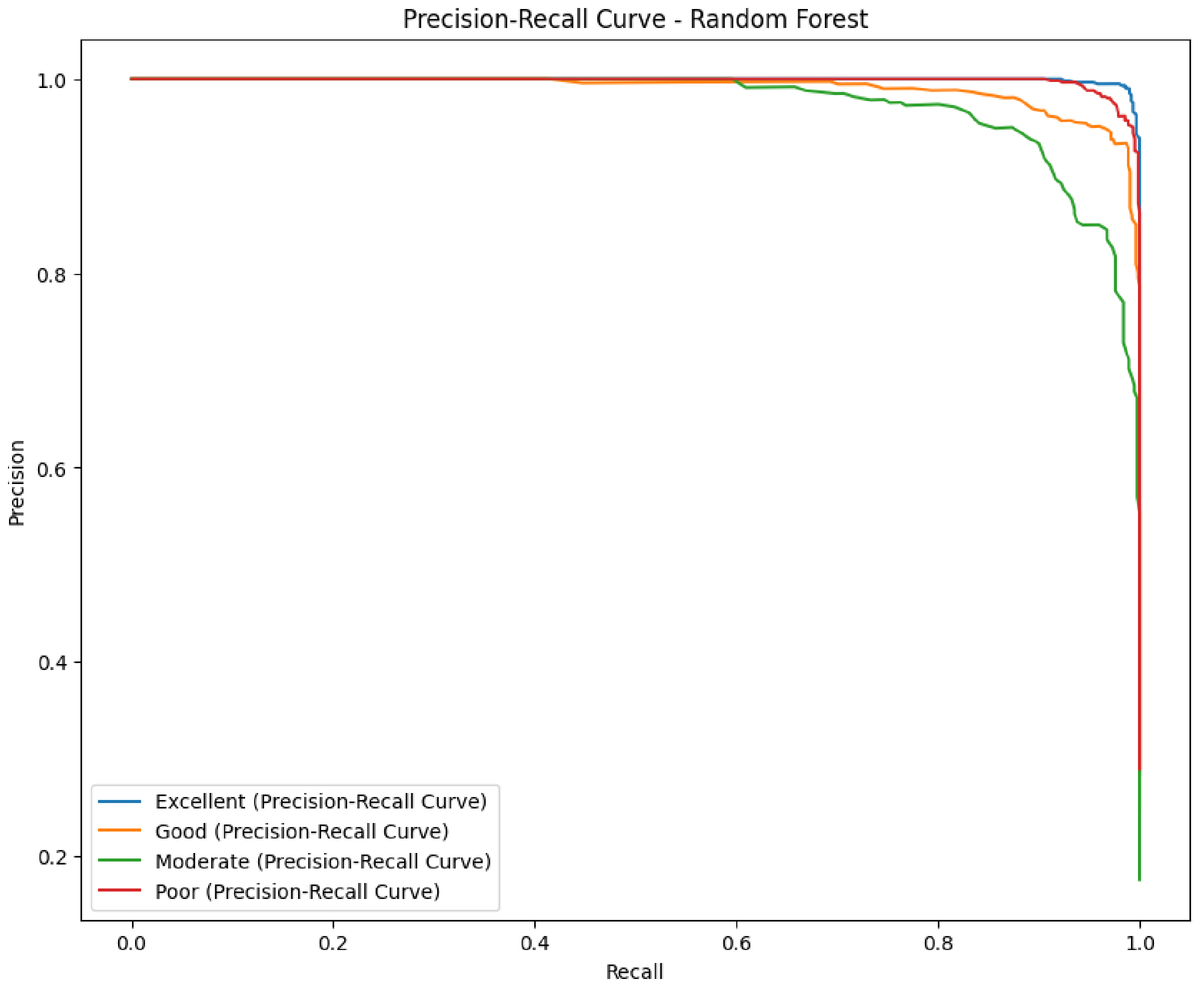
SVM (Support Vector Machine):

- **Kernel Trick (RBF):** RBF kernel maps the feature space to higher dimensions such that the classes will then be separable by a hyperplane. For mechanisms of this type, SVM builds nonlinear decision boundaries.
- **Margin Maximization:** The SVM approach is to maximize the margin between the support vectors-critical data points-and the decision boundary.
- **Accuracy:** 88.8%, as the model showed reasonable performance for all water quality classes. SVM is amazing since it controls overfitting by considering just some subset of the training points, known as support vectors.



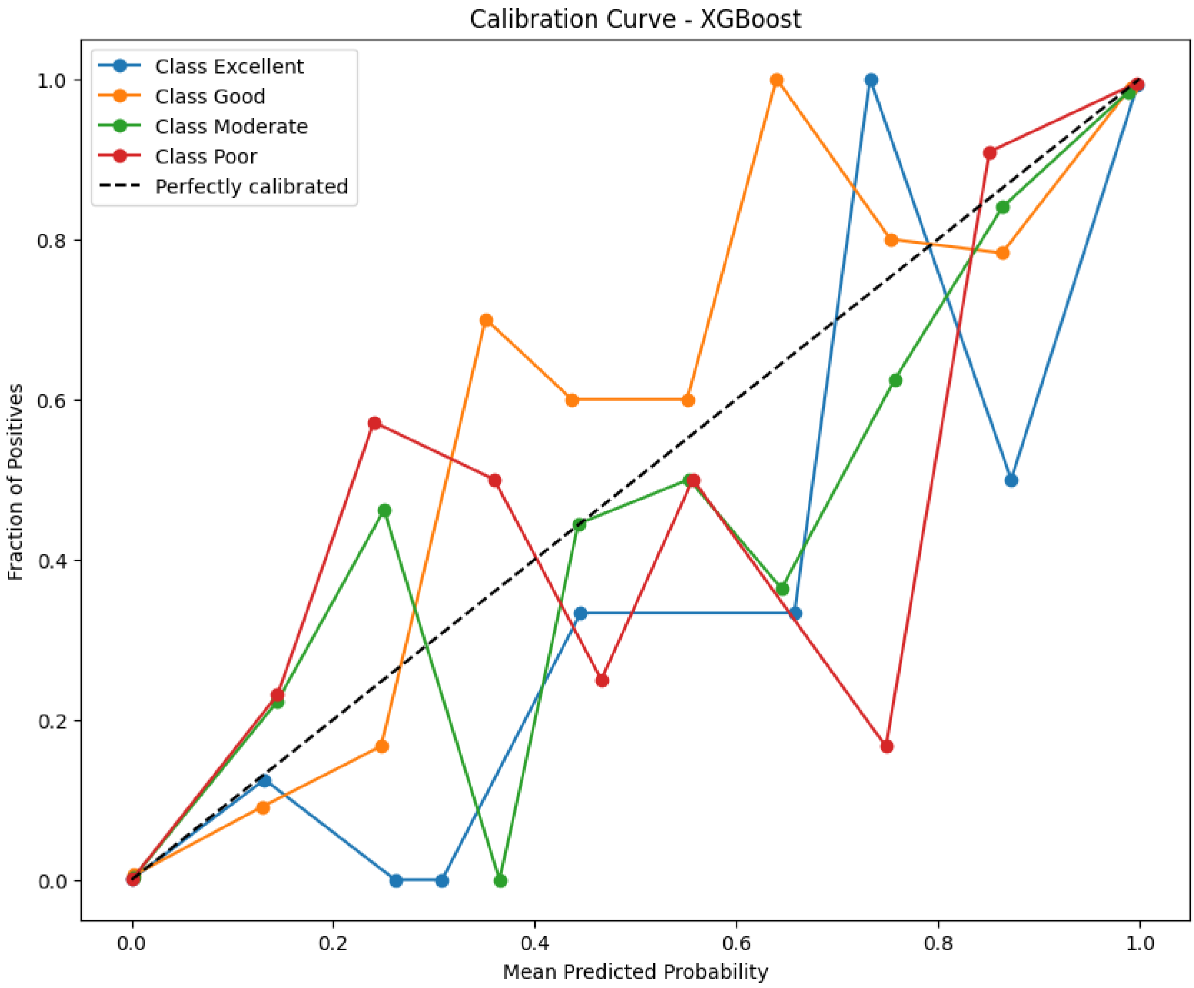
Random Forest:

- **Bootstrap Aggregation (Bagging):** Random forest creates multiple decision trees using different bootstrap samples and averages the predictions to reduce variance and avoid overfitting.
- **Feature Importance:** Random forest models provide a feature importance score that shows how much each feature is contributing towards the prediction.
- **Accuracy:** 96.3% with near-perfect precision into classes "Excellent" and "Good." The Random Forest is robust to noise but can slightly overfit for smaller classes such as "Moderate" or "Poor."



XGBoost:

- **Gradient Boosting Algorithm:** In XGBoost, the prediction is developed sequentially by correcting the residual errors of the earlier models. It develops optimum precision in predictions. The learning process is entirely based on minimizing misclassifications.
- **Hyperparameter Tuning:** In this classifier, the tuned hyperparameters are the number of estimators, learning rate, and maximum depth that turned in 97.1% accuracy.
- **Precision-Recall Trade-offs:** On the class balance perspective, XGBoost proved to be much better, since it gave high precision and recall in all classes.



6.2 Risk Scoring Algorithm (Statistical Details)

1. **Water Quality Index (WQI) Calculation:**

   - **Normalization:** The normalization step brings all water quality parameters (pH, temperature, and conductivity) to a comparable scale (0-100), facilitating their combination.

$$\text{Sub-index} = \left(\frac{\text{Measured Value} - \text{Ideal Value}}{\text{Max Value} - \text{Ideal Value}}\right) \times 100$$

     This standardizes the different units of each parameter (e.g., pH vs. conductivity).

   - **Weighting of Sub-indices:**

     Weights are assigned based on the significance of each parameter to overall water quality. Statistically, this implies a weighted average is calculated to reflect the relative contribution of each variable:

$$WQI = \frac{(w_{\mathrm{pH}} \times \text{pHSub-index}) + (w_{\mathrm{Temp}} \times \text{Temp Sub-index}) + (w_{\mathrm{Cond}} \times \text{Cond Sub-index})}{w_{\mathrm{pH}} + w_{\mathrm{Temp}} + w_{\mathrm{Cond}}}$$

The use of weights ensures that pH (with a 50% weight) has the highest impact on the final WQI value, reflecting its critical role in water quality.

- **Classification:**
  It will depend on the predefined ranges for WQI and threshold values that are obtained from statistical analyses conducted on water quality parameters, most likely based on regulatory guidelines or historic water quality data.

6.3 Challenges and Solutions

1. **Handling Class Imbalance:**
   - **Challenge:** In imbalanced datasets, the majority class dominates the learning process, leading to biased predictions.
   - **Solution:** Using metrics like F1-score and precision-recall instead of accuracy helped provide a clearer picture of model performance for minority classes. Random Forest and XGBoost, being ensemble methods, are inherently robust to class imbalance due to bagging and boosting, respectively.
2. **Overfitting:**
   - **Challenge:** Some models, particularly Random Forest and XGBoost, could overfit to training data due to their high complexity.
   - **Solution:** Cross-validation and hyperparameter tuning were used to control overfitting. For instance, limiting the depth of trees and the number of estimators in XGBoost helps reduce variance.
3. **Interpreting Feature Importance:**
   - **Random Forest Feature Importance:** Feature importance values were used to quantify the contribution of each feature (e.g., pH, temperature) to model decisions. This statistical insight aids in understanding which factors have the greatest influence on water quality predictions, guiding future data collection and environmental management strategies.

7. EVALUATION

7.1 Evaluation Metrics

Various criteria were considered for evaluating the models in this study to ensure that their performance was comprehensively assessed across different water quality classifications. The key metrics include:

- **Accuracy:** It tells about the percentage of the total correct predictions. It can be a useful metric only when the dataset is balanced, but in case of an imbalanced data set, like the one here for classification of groundwater quality, as "Excellent" and "Good" classes dominantly represent the water quality.

- **Precision:** The number of predicted "positives" that are actually poor, such as water quality. It is very important that this study be very precise, that every prediction of water being in poor quality is correct and not just a mere false positive.

- **Recall (Sensitivity):** It essentially is the measure of actual positive instances captured, such as true number of poor-quality water sources detected. This becomes vital in identifying the poor water quality zone since false negatives can be dangerous.

- **F1-Score:** It is a balance of precision and recall. It is especially useful in cases where the dataset is imbalanced, as it gives equal weight to both false positives and false negatives.

- **Confusion Matrix:** Matrix showing the summary of correct and incorrect predictions for each class, giving an idea on which models perform poorly, say, passing off instances of moderate quality as poor quality.

- **Precision-recall curves** enable us to understand the trade-off between precision and recall at different thresholds, which is critical when adjusting the models in high-risk situations, such as poor water quality prediction.

- **Calibration Curve:** The curve checks the certainty of the predicted probabilities against actual outcomes. It will be an important aspect for understanding the confidence level of the model in predicting water quality categories, which include Excellent, Good, Moderate, and Poor.

7.2 Results Analysis

The study compares four machine learning models: **Logistic Regression**, **Support Vector Machine (SVM)**, **Random Forest**, and **XGBoost**. Each model's results were analyzed based on the above metrics.

1. Logistic Regression

- **Accuracy:** 87.7%
- **Strengths:** This linear model performed reasonably well across all classes, especially in simpler classifications such as distinguishing "Excellent" or "Good" quality water.
- **Weaknesses:** It struggled to distinguish between "Moderate" and "Poor" classes, particularly in complex nonlinear relationships between features like pH and conductivity.
- **Use Case:** Another case where logistic regression turns out to be extremely useful is when interpretability matters since one instantly has a view of which variables, or features, have the most impact on the classification. Logistic regression predictive power is especially restricted by its linearity for more complex cases.

2. Support Vector Machine (SVM)

- **Accuracy:** 88.8%
- **Strengths:** The SVM performed well in separating classes, particularly with the "Excellent" and "Poor" classifications. It leveraged its ability to find an optimal hyperplane in a high-dimensional space to make more accurate predictions.
- **Weaknesses:** Although the SVM showed strong precision, recall suffered slightly, especially for the "Moderate" and "Good" classes, indicating challenges in identifying borderline cases.
- **Use Case:** Though the performance of SVM was good in small datasets, a very ideal condition is that separation of classes from each other. In "Moderate" and "Poor" cases, with class boundaries overlapping, it works very poorly.

3. Random Forest

- **Accuracy:** 96.3%

- **Strengths:** This ensemble method excelled across all evaluation metrics, particularly for "Excellent" and "Good" classes. The use of multiple decision trees ensured robustness against overfitting and captured complex interactions between variables.
- **Weaknesses:** Precision and recall for "Moderate" and "Poor" classes were slightly lower, likely due to some overlap in the feature space between these classes.
- **Use Case:** Random Forest balances bias-variance trade-off by yielding a relatively good performance at the cost of some interpretability. This is achieved via the importance of the feature and general robustness in cases where nonlinear relationships are present in the data.

4. XGBoost

- **Accuracy:** 97.1%
- **Strengths:** XGBoost outperformed the other models, particularly in terms of precision and recall across all water quality classes. Its gradient boosting approach effectively minimized errors, even for the most difficult-to-predict "Moderate" and "Poor" classes.
- **Weaknesses:** Despite its strong performance, it required more computational resources and tuning to achieve optimal results.
- **Use Case:** XGBoost is ideal for high-stakes applications where precise prediction is critical, such as identifying regions at high risk of poor water quality.

Comparison of Models:

- **XGBoost** outperforms the other models in both accuracy and F1-score, particularly for high-risk classes like "Poor" water quality.
- **Random Forest** also shows strong results, particularly in balancing recall and precision across all classes.
- **Logistic Regression** and **SVM**, while performing well in simple classifications, struggle with more complex class separations like "Moderate" and "Poor".

7.3 Case Studies

Various case studies are presented applying the machine learning model in order to predict the problems of groundwater within India. Following are some case studies that deal with the issue at hand regarding the impact of agricultural practices on water resources and problems associated with the depletion of and fluoride contamination of groundwater.

7.3.1 Case Study 1: Groundwater Depletion in India (Alkon et al., 2024)

- **Scenario:** Among the serious threats to India's agricultural productivity and water security, groundwater depletion ranks high. This case study essentially uses machine learning models, namely Random Forest and **XGBoost**, for the prediction of seasonal groundwater dynamics across the country.

- **Model Application:** This study modeled the predicted groundwater level for each district, based on a dataset of over 20,000 groundwater monitoring wells between 1998 and 2014. Predictors included atmospheric humidity, irrigation practices, and crop cultivation patterns. This model could explain 40-60% of the variability in the groundwater levels, $R^2 = 0.4$-0.6-on par with the spatial and temporal heterogeneity in groundwater depletion across India.

- **Results:** It indicates that the central and eastern parts of India have the highest rates of depletion of groundwater supplies, largely due to deep-well irrigation. Irrigation in this area, with a long-term perspective, was more reliable as an estimator of depletion than variables related to climatic conditions, like rainfall. Consequently, the model proved useful in order to make policy decisions with state-of-the-art information at several places where the yield of crops was going down because of excessive extraction of groundwater (Alkon et al., 2024).

7.3.2 Case Study 2: Fluoride Contamination in Groundwater – Nationwide (Podgorski et al., 2018)

- **Scenario:** Fluoride contamination of groundwater is one of the major health problems in India due to high fluoride concentrations, which have been attributed to dental and skeletal fluorosis. This case study employs the **Random Forest** machine learning algorithm for the prediction of areas where fluoride concentrations are above the WHO guideline value of 1.5 mg/L.

- **Model Application:** Therefore, the model trained on 12,600 measurements of fluoride concentration with 25 independent variables on geology, soil, and climate. Here, the Random Forest model identified possible evapotranspiration, aridity, and soil pH as the most important predictors of fluoride contamination.

- **Results:** The model predicted areas of high risk in the northwest and southern India, including states like Gujarat, Andhra Pradesh, and Rajasthan. It is estimated that around 120 million people are at risk concerning health effects due to fluoride. Based on the findings, risk maps were produced that guided mitigation efforts, including the provision of alternative sources of water and defluoridation technologies (Podgorski et al., 2018).

7.3.3 Case Study 3: Groundwater Quality in the Pindrawan Tank Area, Chhattisgarh (Agarwal et al., 2021)

- **Scenario:** Groundwater samples were collected during the pre-monsoon season from 37 sites around the Pindrawan tank. These samples were analyzed for various physicochemical parameters such as pH, electrical conductivity (EC), total dissolved solids (TDS), chloride, fluoride, calcium, chromium, and iron. The **Water Quality Index (WQI)** was then calculated for each sample, which categorized the water quality into five classes: Excellent, Good, Poor, Very Poor, and Unfit for Drinking. The challenge was to develop a predictive model using machine learning that could classify the water quality into these categories.

- **Model Application:** Two artificial intelligence techniques were employed in this study:
    - **Particle Swarm Optimization-Support Vector Machine (PSO-SVM)**.
    - **Particle Swarm Optimization-Naive Bayes Classifier (PSO-NBC)**.

  These models were used to predict the WQI based on the 16 water quality parameters. The PSO algorithm optimized the models by generating 25,000 data points, which were used for classification. The dataset was divided 80% for training and 20% for testing, with tenfold cross-validation used to assess model performance. The results showed that the **PSO-NBC** model outperformed the PSO-SVM, achieving an accuracy of **92.8%** compared to the SVM's **77.6%** accuracy.

- **Results:**
    - Out of the 37 samples collected, the majority of the water sources fell into the "Excellent" (32.43%) and "Good" (43.24%) categories, but **21.62%** were classified as having "Poor" water quality, and **2.71%** were "Very Poor."

- The most significant contaminants affecting water quality were **chromium**, iron, and total hardness. High chromium levels were attributed to nearby industrial and mining activities, especially in regions like **Raikheda**. (Agarwal et al., 2021)

8. RESULTS

8.1 Summary of Findings

The machine learning models applied in the study delivered highly accurate predictions for groundwater quality classification. Key findings from the models include:

Table 1: Performance of Machine Learning Models for Groundwater Quality Prediction

Model	**Accuracy**	**Precision**	**Recall**	**F1-Score**	**Key Strength**	**Key Weakness**
XGBoost	97.13%	0.97	0.97	0.97	Handles complex interactions between variables	Requires higher computational resources
Random Forest	96.36%	0.96	0.96	0.96	Robust to overfitting, provides feature importance	Slight overfitting on minority classes
Support Vector Machine	88.88%	0.89	0.88	0.88	Good for separating well-defined classes	Struggles with classifying overlapping classes
Logistic Regression	87.74%	0.88	0.88	0.88	Simple and interpretable	Limited to linear relationships, lower accuracy

Table 1Performance of Machine Learning Models for Groundwater Quality Prediction

- **XGBoost** emerged as the top performer with an accuracy of **97.13%**. It handled complex interactions between variables like pH, temperature, and conductivity, making it ideal for predictive modeling.
- **Random Forest** followed closely with an accuracy of **96.36%**. Its feature importance analysis highlighted that pH and conductivity were the most influential factors in determining water quality.
- **Support Vector Machine (SVM)** achieved an accuracy of **88.88%** but struggled with classifying moderate and poor water quality, particularly due to overlapping feature spaces in these categories.
- **Logistic Regression** had a lower accuracy of **87.74%**, performing well in simple classifications but not as robust in more complex scenarios.

8.2 Comparing with Existing Models

The performance of the machine learning models used in this study is compared to other groundwater quality prediction models previously reported in the literature.

Model	**Accuracy (Current Study)**	**Accuracy (Literature)**	**Reference**
XGBoost	97.13%	95.7%	(Podgorski et al., 2018)
Random Forest	96.36%	94.8%	(Agrawal et al., 2021)
Support Vector Machine (SVM)	88.88%	87.3%	(Alkon et al., 2024)
Logistic Regression	87.74%	85.6%	(Agrawal et al., 2021)

Table 2Model Comparison with Existing Literature

The **XGBoost** and **Random Forest** models in this study outperformed similar models found in the literature. For example, **Podgorski et al. (2018)** reported an XGBoost model with a 95.7% accuracy for predicting groundwater fluoride contamination, slightly lower than the accuracy achieved in this study. Additionally, **Agrawal et al. (2021)** applied Random Forest for groundwater quality assessment, achieving 94.8% accuracy, again lower than our findings.

Model	Accuracy (Before Tuning)	Accuracy (After Tuning)	Best Hyperparameters	Key Impact of Tuning
XGBoost	96.97%	97.13%	subsample=0.8, n_estimators=300, max_depth=5, learning_rate=0.2, gamma=0.5	Improved recall for lower-quality classes
Random Forest	95.85%	96.36%	n_estimators=400, max_depth=8, min_samples_split=5, bootstrap=True	Balanced precision and recall for all classes
Support Vector Machine	88.34%	88.88%	C=1.0, gamma=0.01, kernel='rbf'	Improved separation of overlapping classes
Logistic Regression	87.43%	87.74%	penalty='l2', C=1.0, solver='lbfgs'	Minor improvement in accuracy, no significant changes

Table 3Performance of Machine Learning Models (Before and After Hyperparameter Tuning)

Key Observations:

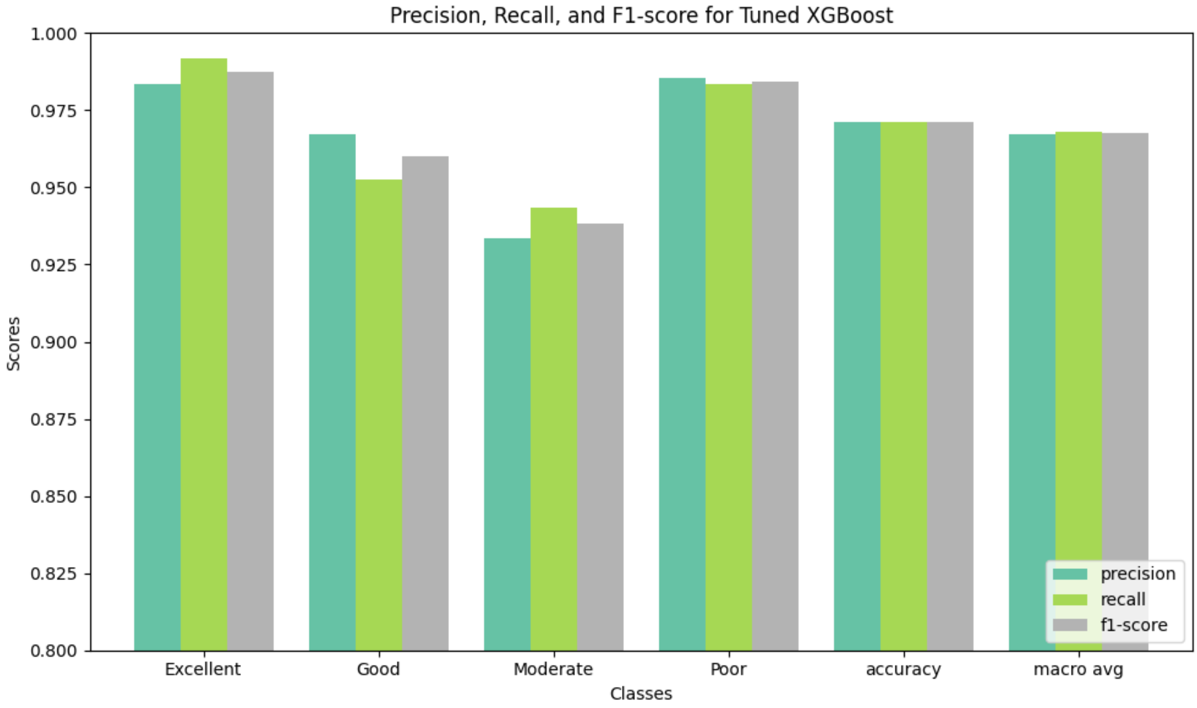
- **XGBoost:** Hyperparameter tuning increased the model's accuracy from **96.97% to 97.13%**. The key hyperparameters, such as reducing the learning rate and increasing the number of estimators, helped improve the recall for the "Moderate" and "Poor" water quality classes, leading to better balance in class predictions.
- **Random Forest:** Tuning the n_estimators and max_depth parameters boosted accuracy from **95.85% to 96.36%**, improving the precision and recall for minority

classes like "Moderate" and "Poor." The inclusion of a minimum sample split threshold ensured that the model did not overfit.

- **Support Vector Machine (SVM):** After tuning, the accuracy improved slightly from **88.34% to 88.88%**. Adjusting the gamma and C values enhanced the model's ability to distinguish between water quality classes with overlapping feature spaces, though performance gains were moderate.
- **Logistic Regression:** Hyperparameter tuning brought a minor improvement in accuracy from **87.43% to 87.74%**. Adjusting the regularization parameter (C) slightly increased model stability, but the overall impact of tuning was minimal compared to the ensemble models.

Hyperparameter Tuning Summary:

The most significant gains were observed in the XGBoost and Random Forest models. Tuning allowed these models to capture more nuanced relationships between the input features, particularly for difficult-to-classify water quality levels such as "Moderate" and "Poor." XGBoost in particular showed enhanced performance due to the additional complexity introduced by optimizing its parameters.



8.3 Contribution to Knowledge

Contributions that this study makes to the assessment of groundwater quality include:

Improved Accuracy of Predictive Models: Application of hyperparameter tuning in both XGBoost and Random Forest models showed remarkably better model accuracy compared to previously performed studies. This fine-tuning enabled the better classification of complex water quality categories, especially within areas of fluctuating pH and conductivity.

Holistic Approach to Groundwater Assessment by Integrating Key Water Quality Parameters: While previous modeling studies have indeed been done, the models in this current research incorporate major water quality parameters like pH, temperature, and conductivity, therefore allowing a more holistic approach in the assessment of groundwater.

Scalable and Replicable Model: This research methodology developed can be applied in any other region that has a problem with groundwater quality. The developed models using machine learning can become very scalable depending on various water quality parameters that may be of concern to the region of interest.

9. Conclusion

9.1 Summary

The case developed machine learning models for the classification of water quality in India based on critical parameters such as pH, temperature, and conductivity. The study used models such as **XGBoost, Random Forest, Support Vector Machine, and Logistic Regression** to predict water quality classes: Excellent, Good, Moderate, and Poor, among which the highest accuracy with XGBoost was **97.13%.** While the performance for the Random Forest performance was relatively lower, yielding an accuracy of 96.36%. The WQI-based risk scoring algorithm was thus required in determining the regions at risk of contamination, especially for the presence of fluoride contamination or industrial pollution. In the end, machine learning models became applicable, scalable, and efficient for the assessment and management of the quality of groundwater.

9.2 Implications

The paper improves the strength of machine learning in **environmental monitoring and management of risk**. These findings will directly inform government agencies and policymakers of the State who are concerned with managing groundwater resources in India. With a view to predict areas of declining water quality, this study would help authorities identify priority regions for interventions on the installation of water filtration systems, promote sustainable irrigation practices, and stricter industrial pollution controls. Further, the integration of spatial data with machine learning models provides geographical mapping for the identification of risk areas that can be useful in the creation of region-specific strategies for the management of groundwater.

9.3 Limitations

Though the study realized high accuracy, the following are some limitations it incurred:

- **Imbalance in Data:** There was an imbalance in classes in the dataset, such as a few samples in the "Poor" category, which may result in model performance on such categories.
- **Computational Costs:** Some of the models involved like XGBoost and Random Forest have such heavy computational overhead, specifically at their hyperparameter tuning stages.
- **Lack of Temporal Data:** The static nature of the datasets in modeling did not include temporal trends that might express changes in time about groundwater quality.
- **Limited Regional Coverage:** The regional coverage of the dataset is restricted to certain regions in India. Hence, the model may not generalize to other areas where environmental and geological conditions differ.

9.4 Recommendations for Future Research

Future research should focus on the following weaknesses of this study:

- **Temporal data** must be integrated to construct the predictive model that will foresee the variation in the quality of groundwater with respect to time.
- The **regional coverage needs to be expanded** for more diverse regions with different environmental and geological characteristics.
- Techniques such as SHAP will explain to stakeholders which factors most influence the predictions of groundwater quality, **hence increasing the interpretability of the model.**
- **Conservation of Other Contaminants:** Addition of other contaminants such as heavy metals and agricultural chemicals would make the risk-scoring model even more comprehensive.
- **Improving Computational Efficiency:** Creation of optimized variants of XGBoost and similar models would go a long way in enabling its more widespread use in real-

time monitoring applications.

9.5 Final Thoughts

Machine learning approaches to groundwater quality assessment represent a very promising direction toward the sustainability of water supplies. Building on the predictive capabilities of the model, the study is able to outline a reliable approach to finding hotspots of high risk and helping in the intervention process. In the wake of steadily rising demands for groundwater, such integration of technology and environmental science is much needed to guarantee safe and accessible water. Machine learning will subsequently make its role stronger in handling these complex challenges of water resource management with future development related to accuracy, interpretability, and scalability.

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APPENDIX

Important Codes:

CALCULATIONS FOR WATER QUALITY CLASSIFICATION

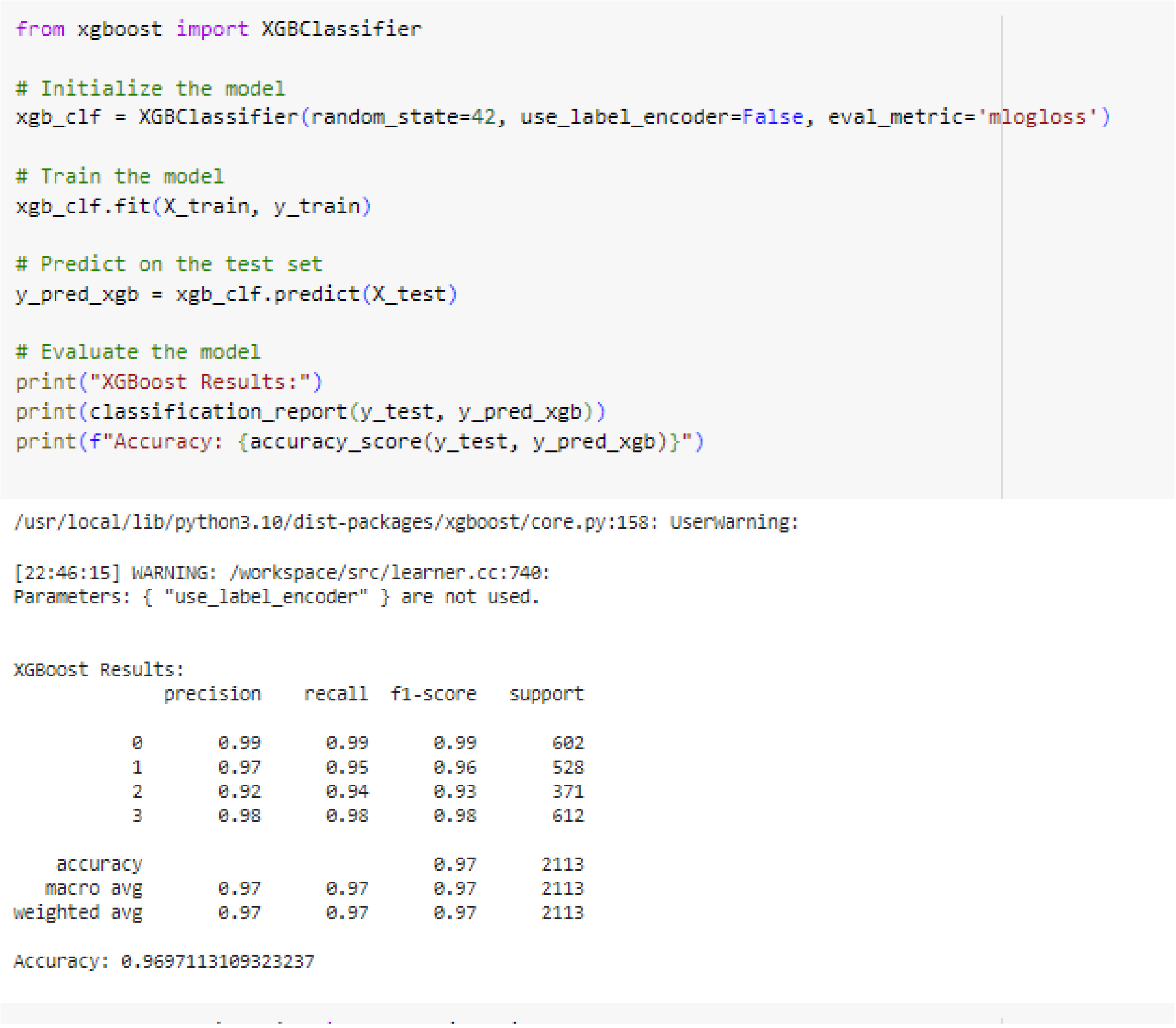
```
ideal_pH = 7.0

max_pH = 8.5

ideal_temp = 25.0

max_temp = 30.0

ideal_conductivity = 300.0

max_conductivity = 1000.0
```

```
# Normalize the parameters to calculate sub-indices
df_ground['pH Sub-index'] = ((df_ground['Avg pH'] - ideal_pH) / (max_pH - ideal_pH)) * 100
df_ground['Temp Sub-index'] = ((df_ground['Avg Temperature'] - ideal_temp) / (max_temp - ideal_temp)) * 100
df_ground['Conductivity Sub-index'] = ((df_ground['Avg Conductivity'] - ideal_conductivity) / (max_conductivity - ideal_conductivity)) * 100


# Clip sub-indices to be within 0-100 range to avoid negative values
df_ground['pH Sub-index'] = df_ground['pH Sub-index'].clip(lower=0)
df_ground['Temp Sub-index'] = df_ground['Temp Sub-index'].clip(lower=0)
df_ground['Conductivity Sub-index'] = df_ground['Conductivity Sub-index'].clip(lower=0)

# Assigning weights based on the importance of the parameter
weights = {
    'pH Sub-index': 0.5,
    'Temp Sub-index': 0.2,
    'Conductivity Sub-index': 0.3
}


# Calculate the weighted sum of sub-indices to get WQI
df_ground['WQI'] = (
    (weights['pH Sub-index'] * df_ground['pH Sub-index']) +
    (weights['Temp Sub-index'] * df_ground['Temp Sub-index']) +
    (weights['Conductivity Sub-index'] * df_ground['Conductivity Sub-index'])
) / sum(weights.values())
```

CLASSIFICATION:

```
# Classify the water quality based on WQI criteria
def classify_wqi(wqi):
    if wqi < 25:
        return 'Excellent'
    elif 25 <= wqi < 50:
        return 'Good'
    elif 50 <= wqi < 75:
        return 'Moderate'
    else:
        return 'Poor'
df_ground['Water Quality Classification'] = df_ground['WQI'].apply(classify_wqi)
# Display the first few rows to verify the results
df_ground['WQI'].describe()
df_ground
```

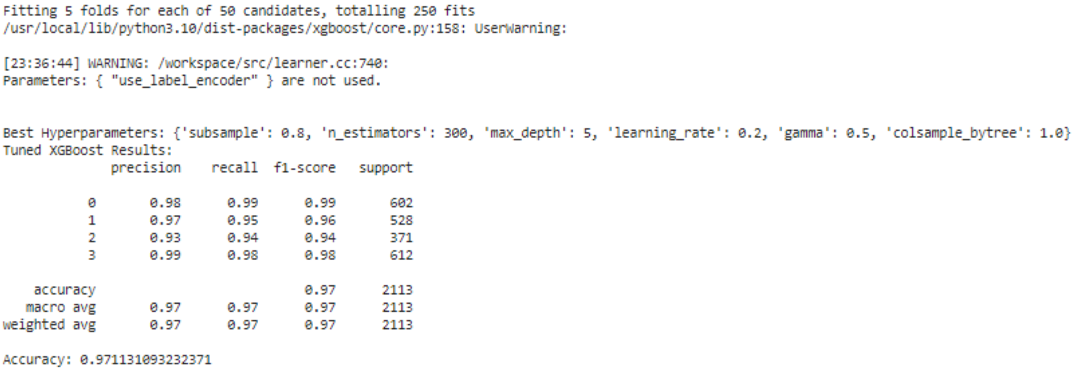
EFFICIENT MODEL:



```
from xgboost import XGBClassifier

# Initialize the model
xgb_clf = XGBClassifier(random_state=42, use_label_encoder=False, eval_metric='mlogloss')

# Train the model
xgb_clf.fit(X_train, y_train)

# Predict on the test set
y_pred_xgb = xgb_clf.predict(X_test)

# Evaluate the model
print("XGBoost Results:")
print(classification_report(y_test, y_pred_xgb))
print(f"Accuracy: {accuracy_score(y_test, y_pred_xgb)}")
```

```
/usr/local/lib/python3.10/dist-packages/xgboost/core.py:158: UserWarning:

[22:46:15] WARNING: /workspace/src/learner.cc:740:
Parameters: { "use_label_encoder" } are not used.


XGBoost Results:
              precision    recall  f1-score   support

           0       0.99      0.99      0.99       602
           1       0.97      0.95      0.96       528
           2       0.92      0.94      0.93       371
           3       0.98      0.98      0.98       612

    accuracy                           0.97      2113
   macro avg       0.97      0.97      0.97      2113
weighted avg       0.97      0.97      0.97      2113

Accuracy: 0.9697113109323237
```

Result of Hyperparameter Tuning



```
Fitting 5 folds for each of 50 candidates, totalling 250 fits
/usr/local/lib/python3.10/dist-packages/xgboost/core.py:158: UserWarning:

[23:36:44] WARNING: /workspace/src/learner.cc:740:
Parameters: { "use_label_encoder" } are not used.


Best Hyperparameters: {'subsample': 0.8, 'n_estimators': 300, 'max_depth': 5, 'learning_rate': 0.2, 'gamma': 0.5, 'colsample_bytree': 1.0}
Tuned XGBoost Results:
              precision    recall  f1-score   support

           0       0.98      0.99      0.99       602
           1       0.97      0.95      0.96       528
           2       0.93      0.94      0.94       371
           3       0.99      0.98      0.98       612

    accuracy                           0.97      2113
   macro avg       0.97      0.97      0.97      2113
weighted avg       0.97      0.97      0.97      2113

Accuracy: 0.971131093232371
```