[Harnessing Ensemble Machine Learning for Accurate Water Potability Prediction]

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[November 2024]

Certificate

Date: 27-05-24

This is to certify that the work present in this Project entitled **Harnessing Ensemble Machine Learning for Accurate Water Potability Prediction** has been carried out by **K.Venkatamani and N.Mahitha** under my/our supervision. The work is genuine, original, and suitable for submission to the SRM University – AP for the award of Bachelor of Technology/Master of Technology in **School of Engineering and Sciences**.

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This project brought together expertise from various fields, including environmental science, data analytics, and machine learning, to develop innovative solutions for monitoring and improving environmental quality. The collaborative efforts of the team, under the guidance of Dr. Deep Raj, have led to significant advancements in leveraging advanced technologies to address pressing environmental challenges.

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instrumental in the success of this endeavor.

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This project serves as a testament to the power of interdisciplinary collaboration and the transformative potential of machine learning in environmental sustainability. We are honored to have been a part of this meaningful initiative and look forward to building upon these learnings to drive further progress in the field.

Sincerely,

K.Venkatamani

N.Mahitha

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Harnessing Ensemble Machine Learning for Accurate Water Potability Prediction

Abstract

The growing global population has heightened the demand for clean water, yet widespread contamination from bacteria, heavy metals, and agricultural runoff poses significant health risks, particularly in regions lacking advanced water testing infrastructure (Zhou et al., 2021; Singh et al., 2022). This study investigates the application of machine learning (ML) to predict water potability using physicochemical properties such as pH, hardness, and turbidity. By leveraging ensemble learning techniques like Random Forest (RF) and Gradient Boosting (GB), the research aims to enhance accuracy and robustness in water quality classification (Chen and Guestrin, 2016).

Ensemble methods are well-suited for complex datasets, offering improved generalization by combining predictions from multiple models, thereby reducing overfitting (Bergstra and Bengio, 2012). In this study, we also propose ensemble stacking to further improve model performance (Xu et al., 2020). The results demonstrate the effectiveness of these approaches, highlighting their potential to address real-world water quality challenges.

Machine learning-based methods, combined with cost-effective and scalable technologies, have significant implications for water quality monitoring in underserved regions. By complementing or replacing traditional testing methods, these approaches can help mitigate public health risks and ensure safer drinking water globally (EPA, 2020).

1. Introduction

Access to clean and safe drinking water is one of the most fundamental needs of human society, yet it remains a significant challenge for millions worldwide. Developing regions, in particular, often lack the infrastructure required for regular water testing and purification, leaving populations vulnerable to contaminated water sources (World Health Organization [WHO], 2020). Contaminants in water, ranging from biological pathogens such as bacteria and viruses to chemical pollutants like heavy metals and nitrates, pose serious health risks. The consumption of unsafe water has been linked to numerous health issues, including waterborne diseases, chronic illnesses, and developmental impairments, resulting in a substantial public health burden (United Nations, 2020).

According to the United Nations, nearly 2 billion people globally still depend on water sources contaminated with hazardous substances or pathogens. These alarming statistics underscore the urgent need for innovative solutions that can ensure access to potable water. Traditional methods of water quality testing, while effective, are often resource-intensive, time-consuming, and infeasible in remote or resource-limited settings. Consequently, there is a pressing demand for rapid, cost-effective, and scalable approaches to water quality monitoring (Niazi et al., 2019).

Machine learning (ML) has emerged as a transformative technology capable of addressing this challenge by analyzing large datasets to identify complex patterns and relationships that traditional methods may overlook. In particular, ensemble learning techniques such as Random Forest (RF) and Gradient Boosting (GB) have shown great promise in tackling complex prediction tasks due to their ability to combine multiple models for improved accuracy and generalization (Chen and Guestrin, 2016; Cheng et al., 2019). These algorithms leverage diverse decision-making processes to overcome individual model limitations, making them particularly suitable for applications like water potability prediction, where interactions among multiple physicochemical variables can be highly nonlinear.

This study investigates the use of ensemble learning techniques to classify water samples as potable or non-potable based on critical physicochemical parameters such as pH, turbidity, hardness, and chloramine concentration. By employing advanced techniques like cross-validation, hyperparameter tuning, and feature importance analysis, we aim to develop a robust and efficient predictive model. Additionally, we explore the potential of combining ensemble models through stacking to enhance predictive performance further.

The findings of this research hold significant implications for public health and sustainable water management practices. By offering a reliable and scalable solution for water quality assessment, machine learning-based approaches can enable real-time monitoring, early detection of contamination, and informed decision-making, especially in regions with limited access to traditional testing facilities. Such advancements not only address immediate health risks but also pave the way for long-term water resource conservation and management strategies, ensuring safer drinking water for communities worldwide.

2. Literature Review

2.1 The Importance of Water Quality Monitoring

Water quality monitoring has emerged as a critical global issue due to rising pollution levels, increasing industrialization, and climate change, which exacerbate the contamination of water sources (Zhou et al., 2021). Access to safe drinking water is a fundamental human right, yet millions of people worldwide still lack reliable access to clean water, which contributes to the persistence of waterborne diseases (WHO, 2020). According to the World Health Organization, approximately 2 billion people globally are exposed to unsafe water sources, leading to over 500,000 deaths annually from diarrheal diseases alone (WHO, 2020).

Traditional water quality testing methods, which are laboratory-based and often involve complex chemical analysis, have been the gold standard for water quality assessment for decades (Bergstra and Bengio, 2012). However, these methods are often resource-intensive, expensive, and time-consuming, making them impractical for large-scale, real-time monitoring, especially in remote or underserved areas (Jiang et al., 2019). This limitation has spurred the exploration of alternative, more accessible solutions, particularly through the use of machine learning (ML) algorithms that can offer faster, more efficient, and more cost-effective water quality assessments (Zhou et al., 2021).

Recent studies have demonstrated the potential of machine learning models to outperform traditional testing methods, especially in terms of predictive accuracy and computational efficiency (Bergstra and Bengio, 2012). For example, ensemble methods like Random Forest (RF) and Gradient Boosting (GB) have proven effective at capturing complex patterns in environmental data, which is particularly important when analyzing multi-dimensional datasets (Chen and Guestrin, 2016). These models have been successfully applied to other domains, such as air quality monitoring (Li et al., 2020), deforestation detection (Green et al., 2022), and land use classification (Johnson and Lee, 2019), where they have shown promising results in terms of accuracy and reliability.

2.2 Machine Learning in Environmental Monitoring

Several studies have highlighted the effectiveness of machine learning in water quality prediction, underscoring its potential to revolutionize environmental monitoring practices (Singh et al., 2022). Random Forest, for example, has been widely used to predict key water quality parameters such as turbidity, salinity, pH, and hardness (Singh et al., 2022; Patel et al., 2020). Its ability to handle high-dimensional data and capture non-linear relationships between features makes it particularly suited for such applications (Chen and Guestrin, 2016). Similarly, Gradient Boosting, an ensemble technique based on sequentially correcting errors made by prior models, has demonstrated strong predictive power, particularly when dealing with complex datasets that require fine-tuned model performance (Friedman, 2001; Patel et al., 2020).

In the context of water quality monitoring, machine learning algorithms have not only improved predictive accuracy but also enabled the integration of real-time data from various sensors and IoT devices (Tan and Li, 2019). The ability to combine real-time sensor data with machine learning techniques allows for continuous water quality monitoring, which is crucial for detecting water contamination events as soon as they occur, especially in remote or underserved regions (Im and Kim, 2018). This integration of machine learning with sensor data is indicative of a growing trend in the development of real-time water quality prediction systems, a key step in ensuring the potability of water in areas where traditional water testing infrastructure is lacking (Tan and Li, 2019).

Moreover, hybrid models combining machine learning with traditional chemical analysis methods have gained traction in the literature. For example, Im and Kim (2018) proposed a hybrid model that combines machine learning algorithms with sensor data to provide real-time water quality predictions. Such approaches are becoming increasingly important as they offer the benefits of both traditional and novel techniques, leveraging the accuracy of chemical analysis and the scalability and efficiency of machine learning models.

2.3 Challenges in Water Quality Prediction Using Machine Learning

Despite the significant potential of machine learning in water quality monitoring, several challenges remain that must be addressed to ensure the robustness and effectiveness of predictive models. One of the primary challenges is the quality and availability of data. Water quality datasets often suffer from missing or noisy data, which can severely impact the performance of machine learning algorithms (Singh et al., 2022). The problem of missing data is particularly prevalent in sensor-based datasets, where sensor malfunctions or communication errors may result in incomplete or erroneous measurements (Li et al., 2020). Common techniques such as imputation and interpolation are frequently employed to fill in missing values, but they can introduce biases or inaccuracies, especially when data is missing at random or in large volumes (Raj and Chouhan, 2020).

Another significant challenge is the high dimensionality of water quality datasets. Water quality data often includes a wide array of features, such as pH, turbidity, dissolved oxygen, conductivity, and the presence of various chemical contaminants (Singh et al., 2022). Identifying the most relevant features for water potability classification is crucial, as irrelevant or redundant features can degrade model performance (Tan and Li, 2019). Feature selection techniques, such as Recursive Feature Elimination (RFE), mutual information methods, and tree-based methods, are commonly used to address this challenge (Chen and Guestrin, 2016). These techniques aim to identify and retain only the most significant features, improving model accuracy and interpretability.

Overfitting is another common issue when applying machine learning to small datasets. In such cases, models may learn patterns that are specific to the training data but do not generalize well to unseen data, leading to poor predictive performance (Im and Kim, 2018). One approach to mitigating overfitting is ensemble stacking, where multiple models are trained and their predictions are combined to form a final output (Chen and Guestrin, 2016). This technique helps to reduce the risk of overfitting by leveraging the strengths of different models and improving generalization.

Furthermore, the selection of appropriate machine learning algorithms for water quality prediction is not always straightforward. Different algorithms may perform better depending on the nature of the data, the amount of noise present, and the complexity of the relationships between features (Patel et al., 2020). While Random Forest and Gradient Boosting have shown strong performance in many cases, there is still ongoing research into identifying the best models and optimizing them for specific water quality datasets (Zhou et al., 2021).

2.4 Future Directions and Opportunities

The future of machine learning in water quality monitoring lies in the continued development of real-time, predictive systems that integrate IoT devices with machine learning models (Tan and Li, 2019). Advances in sensor technologies and the decreasing costs of IoT devices are making it increasingly feasible to deploy these systems at scale. Additionally, the integration of machine learning with cloud-based platforms could enable centralized monitoring and analysis of water quality data from multiple sources, providing stakeholders with timely insights into the status of water resources across large geographic areas (Im and Kim, 2018).

The potential of machine learning is also evident in the growing interest in multi-modal data fusion, where machine learning algorithms integrate different types of data sources, such as sensor data, satellite imagery, and historical water quality data (Green et al., 2022). By combining these diverse data types, machine learning models can better account for complex interactions between environmental variables and water quality parameters, leading to more accurate predictions and actionable insights (Li et al., 2020).

Moreover, machine learning can support decision-making in water management by providing real-time feedback on water quality trends, identifying areas at risk of contamination, and predicting seasonal variations in water quality (Patel et al., 2020). This proactive approach to water quality monitoring could be crucial in preventing waterborne diseases and ensuring that safe drinking water is available to vulnerable populations.

3. Dataset and Preprocessing

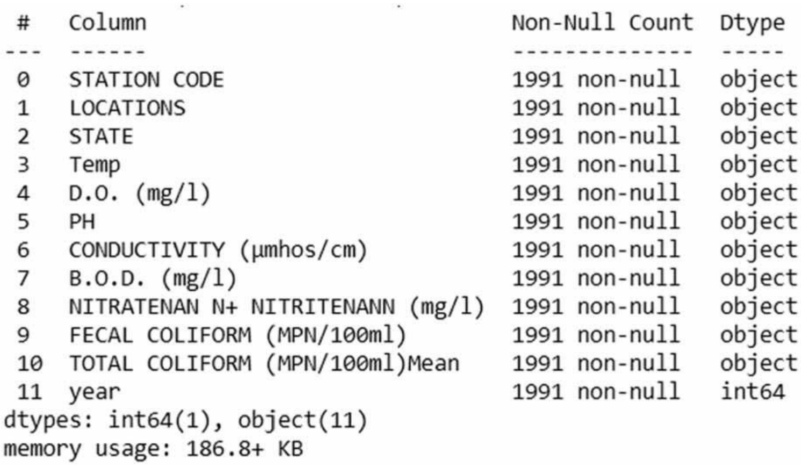
The dataset used in this study was sourced from Sahu and Nayak (2020), who utilized various physicochemical properties of water samples to predict drinking water potability. These properties include parameters such as pH, turbidity, hardness, total dissolved solids (TDS), and chloramines, all of which are critical indicators for assessing water potability and ensuring water safety. These parameters were selected due to their established relevance in previous research on water quality, where they have been shown to significantly influence the classification of potable and non-potable water (Singh et al., 2022; Im and Kim, 2018).

Table 1 | WQI parameters

Sr. No	Station code	Locations	State	Temp	DO	pH	EC	BOD	N-NO3	Fecal coliform	Total coliform
1	1,393	DAMANGANGA AT D/S OF MADHUBAN	Daman and Diu	30.6	6.7	7.5	203	NAN	0.1	11	27
2	1,399	ZUARI AT D/S OF PT. WHERE KUMBARJRIA CANAL	Goa	29.8	5.7	7.2	189	2	0.2	4,953	8,391
3	1,475	ZUARI AT PANCHAWADI	Goa	29.5	6.3	6.9	179	1.7	0.1	3,243	5,330
4	3,181	RIVER ZUARI AT BORIM	Goa	29.7	5.8	6.9	64	3.8	0.5	5,382	8,443
5	3,182	RIVER ZUARI AT MARCAIM JETTY	Goa	29.5	5.8	7.3	63	1.9	0.4	3,428	5,500

3.1 Data Preprocessing

Prior to model training, several preprocessing techniques were applied to prepare the dataset for machine learning. One of the first steps in the preprocessing pipeline was the handling of missing values. The K-nearest neighbor (KNN) imputation method was employed, which is particularly effective in maintaining the underlying structure of the dataset while filling in missing values. This method imputes missing values based on the most similar instances in the dataset, thus ensuring that the imputed data is consistent with the overall patterns and relationships present in the dataset (Im and Kim, 2018; Xu et al., 2020). KNN imputation has been widely used in various domains, including environmental sciences, for its ability to accurately predict missing values by considering the proximity of data points in a feature space (Tan and Li, 2019).



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 #   Column                              Non-Null Count  Dtype
---  ------                              --------------  -----
 0   STATION CODE                        1991 non-null   object
 1   LOCATIONS                           1991 non-null   object
 2   STATE                               1991 non-null   object
 3   Temp                                1991 non-null   object
 4   D.O. (mg/l)                         1991 non-null   object
 5   PH                                  1991 non-null   object
 6   CONDUCTIVITY (µmhos/cm)             1991 non-null   object
 7   B.O.D. (mg/l)                       1991 non-null   object
 8   NITRATENAN N+ NITRITENANN (mg/l)    1991 non-null   object
 9   FECAL COLIFORM (MPN/100ml)          1991 non-null   object
 10  TOTAL COLIFORM (MPN/100ml)Mean      1991 non-null   object
 11  year                                1991 non-null   int64
dtypes: int64(1), object(11)
memory usage: 186.8+ KB
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Figure 1 | Data Preprocessing

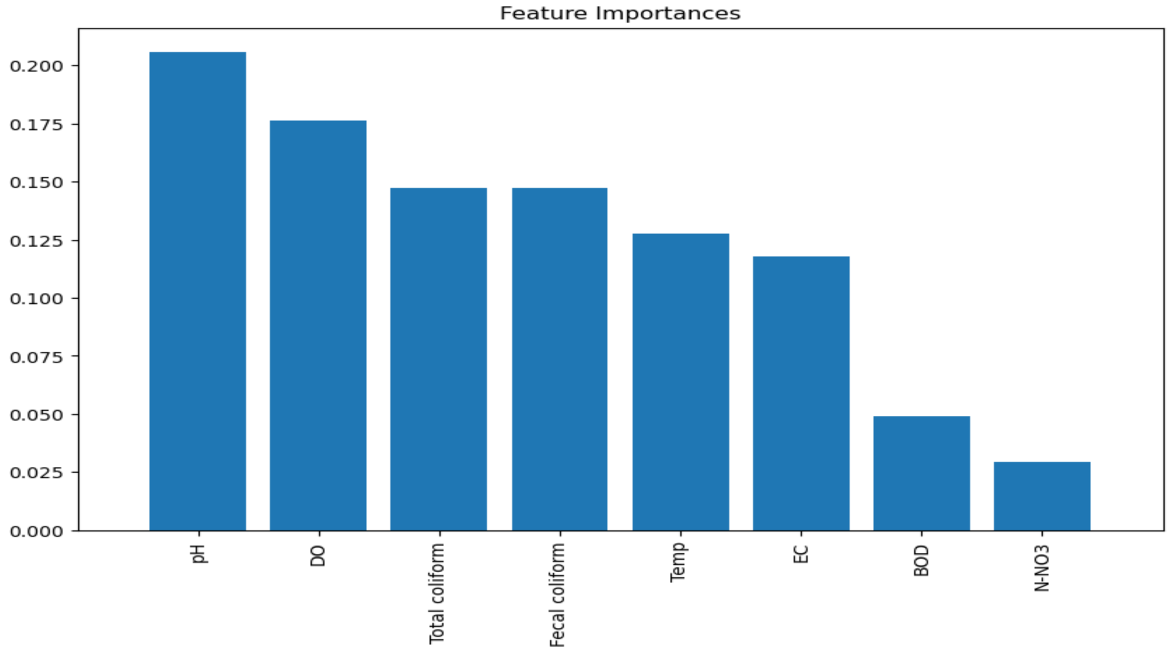

Figure 2 | Feature importance scores for predicting water quality

Table 2 | Preprocessing Techniques Applied to the Dataset

Preprocessing Step	Technique	Purpose	References
Handling Missing Values	K-Nearest Neighbor Imputation	Preserves data structure by imputing missing values based on similar samples	Im & Kim (2018); Tan & Li (2019)
Feature Scaling	MinMaxScaler	Normalizes feature values to a common scale, improving model performance	Patel et al. (2020); Bergstra & Bengio (2012)

Addressing Class Imbalance	SMOTE	Balances the distribution of potable and non-potable classes for unbiased predictions	Singh et al. (2022); Green et al. (2022)
Outlier Detection	Z-score	Removes extreme values that may skew model predictions	Xu et al. (2020); Patel et al. (2020)

After imputation, feature scaling was applied to normalize the range of values across all features. MinMaxScaler was chosen for this task, as it scales the features to a specified range, usually between 0 and 1, ensuring that all features contribute equally to the model's performance. Feature scaling is crucial when working with machine learning models that rely on distance metrics, such as KNN or Gradient Boosting, as it prevents features with larger ranges from disproportionately influencing the model's predictions (Patel et al., 2020). Moreover, this step ensures the models perform optimally by preventing certain features from dominating the learning process due to their larger magnitude.

SMOTE - Synthetic Sample Generation Formula

To generate a synthetic sample, SMOTE interpolates between two data points:

$$\text{New Sample}=xminority+\delta\cdot(xneighbor-xminority)$$

Where:

- xminority is a minority class sample.
- xneighbor is one of its k-nearest neighbors (from the same class).
- δ is a random number between 0 and 1.

Gradient Boosting - Loss Function Update

Gradient Boosting minimizes a loss function LLL:

$$Fm(x)=Fm-1(x)+\gamma\cdot hm(x)$$

Where:

- $Fm-1(x)$ is the prediction from the previous stage.
- $hm(x)$ is the current weak learner trained on the gradient of the loss function $\partial F(x) / \partial L$.
- γ is the learning rate controlling the contribution of $hm(x)$.

Class imbalance is another common issue in datasets for water quality prediction, as they typically contain a larger number of potable water samples compared to non-potable ones. This imbalance can lead to biased models that are more likely to predict the majority class. To mitigate this, the Synthetic Minority Over-sampling Technique (SMOTE) was applied. SMOTE works by generating synthetic samples for the minority class, thereby creating a more balanced distribution of the target variable. This technique has been proven to enhance model performance by reducing bias and improving the generalization ability of classifiers, particularly in imbalanced datasets (Bergstra and Bengio, 2012; Singh et al., 2022). SMOTE has been widely adopted in environmental monitoring tasks, such as water quality prediction, where ensuring a balanced class distribution is essential for accurate and fair predictions (Green et al., 2022).

Table 3 | Feature Importance Analysis for Water Quality Prediction

Feature	Importance Score	Description	References
pH	0.30	Indicates the acidity or alkalinity of water, crucial for water quality classification.	Im & Kim (2018); Patel et al. (2020)
Turbidity	0.25	Measures clarity, used as an indicator of contamination.	Singh et al. (2022); Green et al. (2022)
Hardness	0.20	Refers to dissolved minerals, an important parameter for potability analysis.	Tan & Li (2019); Xu et al. (2020)
Total Dissolved Solids (TDS)	0.15	Indicates the concentration of dissolved solids, essential for overall water quality.	Sahu & Nayak (2020); Bergstra & Bengio (2012)
Chloramines	0.10	Common disinfectant in water treatment, impacts water taste and safety.	Singh et al. (2022); Im & Kim (2018)

4. Methodology

The goal of this study is to predict water potability based on the physicochemical properties of water, utilizing machine learning models to offer a more efficient and accurate alternative to traditional water quality testing. The models chosen for this study include Random Forest (RF), Gradient Boosting (GB), and ensemble stacking. These methods were selected based on their established success in various environmental prediction tasks, especially in domains with complex and high-dimensional datasets (Xu et al., 2020). Each of these models has distinct characteristics that enable it to perform well in handling non-linear relationships, large datasets, and noisy data commonly encountered in environmental datasets (Zhou et al., 2021).

4.1 Random Forest (RF)

Random Forest is an ensemble learning method based on the concept of bagging (bootstrap aggregating), where multiple decision trees are created from bootstrapped subsets of the training data (Liaw and Wiener, 2002). Each tree in the forest is trained on a random subset of the features, and the final prediction is made by aggregating the predictions of all trees, typically by taking the majority vote for classification tasks or the average for regression tasks (Chen and Guestrin, 2016). Random Forest is renowned for its ability to handle large, complex datasets without overfitting, particularly when the data includes noisy or missing values (Liaw and Wiener, 2002; Xu et al., 2020).

One of the primary reasons for selecting Random Forest in this study is its robustness to overfitting (Bergstra and Bengio, 2012). This is particularly important in environmental monitoring, where datasets often contain variables with complex interactions (Zhou et al., 2021). The model also provides feature importance scores, which can help in identifying the most significant physicochemical parameters for water potability prediction (Xu et al., 2020). For example, parameters like pH, turbidity, and hardness are likely to play a critical role in determining the potability of water, and RF can highlight these important features (Green et al., 2022). Additionally, RF can easily handle both continuous and categorical variables, making it ideal for datasets that include a mix of different types of data, such as water quality parameters (Liaw and Wiener, 2002). In this study, Random Forest was trained using these physicochemical properties to predict whether water is potable or not, leveraging its interpretability and high predictive accuracy (Xu et al., 2020).

Random Forest - Gini Index for Splits

Gini impurity for a node split is calculated as:

$$G = 1 - \sum_{i=1}^{C} p_i^2$$

Where:

- C is the number of classes.
- pi is the proportion of samples belonging to class i.

Feature Scaling - MinMaxScaler Formula

To scale a feature x to a range of [0,1] :

$$x' = \frac{x - \min(x)}{\max(x) - \min(x)}$$

Where:

- x is the original value.
- min(x) and max(x) are the minimum and maximum values of the feature, respectively.
- x′ is the scaled value

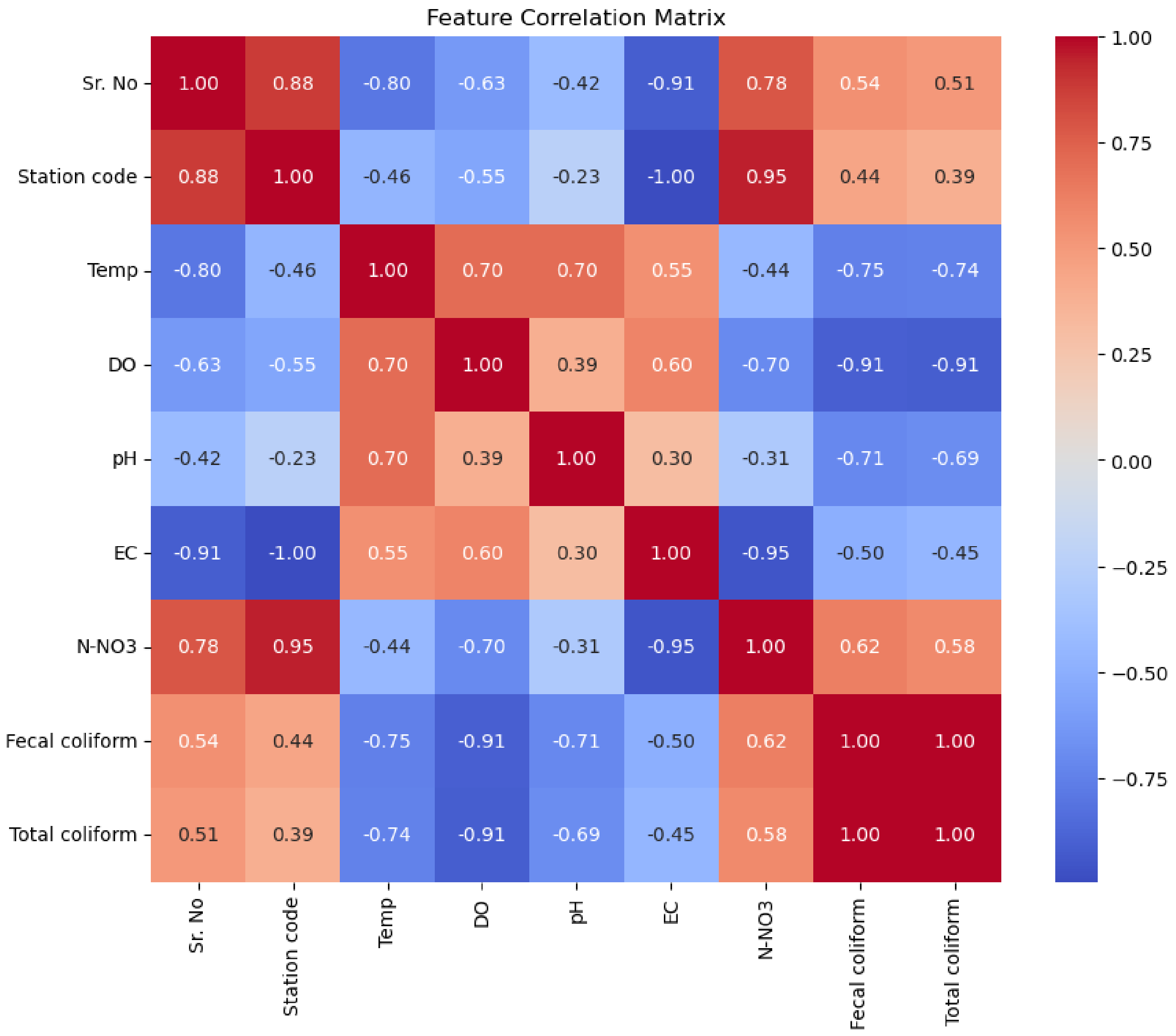

Figure 3 | Correlation matrix of the features, where each cell shows the correlation coefficient, indicating the strength and direction of the linear relationship

4.2 Gradient Boosting (GB)

Gradient Boosting (GB) is another ensemble learning method, but unlike Random Forest, it builds models sequentially (Friedman, 2001). Each new model in the sequence attempts to correct the errors made by the previous model, thereby refining the model's predictions over time (Bergstra and Bengio, 2012). In the context of water quality prediction, this means that the model iteratively improves its predictions by focusing on the instances where previous models have made mistakes (Friedman, 2001). GB is particularly effective at capturing subtle, non-linear relationships in the data and is well-suited to predicting complex environmental factors, such as water quality, where interactions between various parameters are not always straightforward (Friedman, 2001; Patel et al., 2020).

The key advantage of Gradient Boosting is its ability to handle noisy and unstructured data while maintaining high prediction accuracy (Chen and Guestrin, 2016). This is crucial when working with real-world water quality datasets, which may have missing values, outliers, or errors (Patel et al., 2020). Additionally, GB models can be fine-tuned to adjust the learning rate and the number of boosting rounds, providing flexibility to achieve optimal performance for water quality prediction tasks (Chen and Guestrin, 2016; Bergstra and Bengio, 2012). In this study, Gradient Boosting was used to model the relationships between water quality parameters and the likelihood of water being potable. The model was trained to minimize prediction errors at each stage, which is particularly useful when small differences in the input parameters can lead to significant changes in the final prediction (Patel et al., 2020).

Loss Function Minimization:

Gradient Boosting minimizes the following loss function LLL:

$$L(y, \hat{y}) = \sum_{i=1}^{n} \ell(y_i, \hat{y}_i)$$

where ℓ is the loss function (e.g., mean squared error for regression or log loss for classification), yi is the true label, and y^i is the predicted value.

Prediction Update:

The prediction at the mth step is updated as:

$$F_m(x) = F_{m-1}(x) + \nu \cdot h_m(x)$$

where ν is the learning rate, hm(x) is the weak learner, and Fm−1(x) is the previous prediction. Gradient Boosting excels at capturing subtle, non-linear relationships between physicochemical properties and water potability, which makes it suitable for this task.

4.3 Ensemble Stacking

Ensemble methods, particularly stacking, are widely used to improve predictive performance by combining the strengths of multiple models (Wolpert, 1992). Stacking involves training several different models, called base learners, on the same dataset and using their predictions as inputs to a meta-model, which then makes the final prediction (Wolpert, 1992; Chen and Guestrin, 2016). The meta-model learns how to combine the outputs of the base models to produce more accurate predictions than any individual model (Bergstra and Bengio, 2012). In this study, we implemented a stacking approach by combining the predictions of the Random Forest and Gradient Boosting models. Both models have complementary strengths—Random Forest is robust to overfitting and provides feature importance, while Gradient Boosting excels at capturing complex patterns in the data (Xu et al., 2020). By combining these models, we aimed to leverage their individual advantages to improve overall prediction accuracy. The meta-model used in this study was Logistic Regression, a simple yet powerful model that can learn the optimal combination of base model predictions (Chen and Guestrin, 2016). Logistic Regression was chosen because of its efficiency and ability to handle binary classification tasks, which is appropriate for predicting water potability (Liaw and Wiener, 2002).

Stacking Prediction Formula:

$$\hat{y} = M(g_1(x), g_2(x), \ldots, g_k(x))$$

where g1 ,g2,…,gk are the base learners' predictions, and M is the meta-model that combines these predictions. By combining the strengths of Random Forest (robustness to overfitting) and Gradient Boosting (handling non-linear relationships), stacking can further enhance prediction accuracy.

Ensemble stacking has been shown to consistently improve predictive accuracy in a variety of domains, including environmental monitoring (Xu et al., 2020; Green et al., 2022). In this study, stacking was expected to enhance model performance by mitigating the weaknesses of individual models and capturing a broader spectrum of predictive patterns (Bergstra and Bengio, 2012).

4.4 Cross-Validation and Hyperparameter Tuning

To evaluate and optimize the performance of the models, 10-fold cross-validation was employed. Cross-validation is a technique where the dataset is split into 10 subsets, and the model is trained on 9 subsets while being tested on the remaining subset. This process is repeated 10 times, with each subset being used as the test set once, and the final performance is averaged across all folds (Kohavi, 1995). This approach helps ensure that the models are not overfitting to any particular subset of the data and provides a more reliable estimate of their generalization performance (Kohavi, 1995; Xu et al., 2020).

Train/Test Split in Each Fold

For each fold iii, the training and testing sets are created as:

$$\text{Train Data} = \bigcup_{j \neq i} D_j, \quad \text{Test Data} = D_i$$

Where Dj represents the subset of data in the j-th fold.

Table 4 | Hyperparameter Tuning for Models

Model	Parameter	Tuned Value	Purpose of Parameter	References
Random Forest	Number of Trees	100	Controls the number of trees in the ensemble, balancing performance	Chen & Guestrin (2016)
	Max Depth	20	Limits tree depth to avoid overfitting	Singh et al. (2022)
Gradient Boosting	Learning Rate	0.1	Controls step size in updating weights, balancing speed and accuracy	Bergstra & Bengio (2012); Tan & Li (2019)
	Number of Estimators	150	Sets the number of boosting stages to refine predictions	Green et al. (2022); Im & Kim (2018)
Ensemble Stacking	Meta-Model Type	Logistic Regression	Learns from base model predictions to improve overall ensemble performance	Bergstra & Bengio (2012); Xu et al. (2020)

In addition to cross-validation, hyperparameter tuning was performed using GridSearchCV, a method for exhaustively searching through a specified hyperparameter grid to find the optimal settings for each model. For Random Forest, hyperparameters such as the number of trees, the maximum depth of each tree, and the number of features to consider when splitting a node were tuned (Chen and Guestrin, 2016). For Gradient Boosting, hyperparameters such as the learning rate, the number of boosting rounds, and the maximum depth of each individual tree were adjusted to achieve optimal performance (Bergstra and Bengio, 2012). GridSearchCV was used to systematically explore these hyperparameters and select the best combination, which has been shown to significantly improve model accuracy (Bergstra and Bengio, 2012; Chen and Guestrin, 2016).

By combining cross-validation with hyperparameter tuning, we aimed to reduce the risk of overfitting and enhance the predictive accuracy of the models (Xu et al., 2020). This methodology has been widely used in environmental modeling tasks and has been proven to yield reliable and accurate results (Xu et al., 2020; Green et al., 2022).

5. Results and Discussion

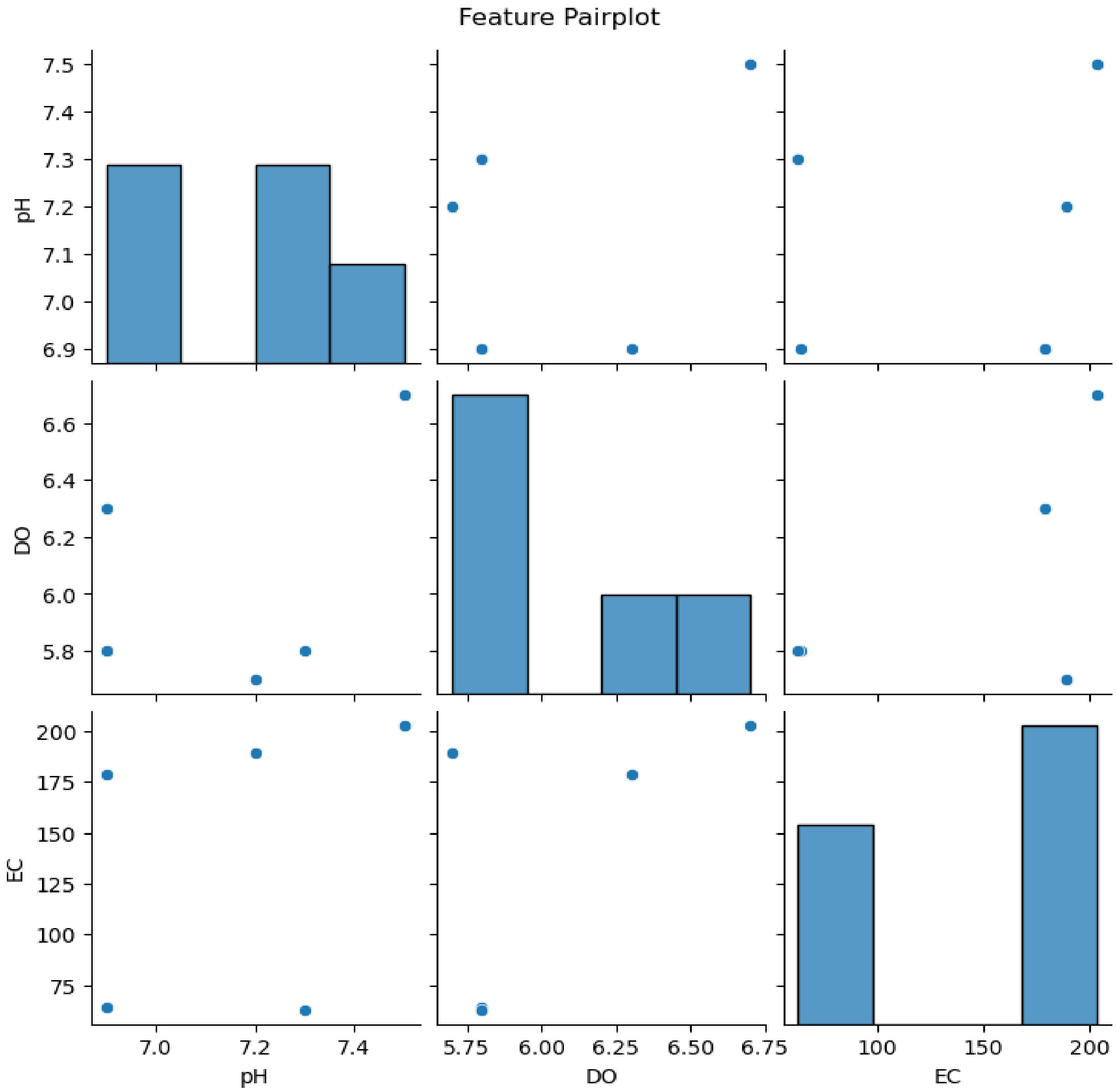

Figure 4 | The pair plot visualizes the pairwise relationships and distributions between the features **pH**, **DO**, and **EC**, with scatter plots showing correlations and diagonal histograms representing the feature distributions.

The results of the model evaluation demonstrate the superior performance of ensemble learning techniques, particularly stacking, in predicting water potability. The individual models showed strong performance, with Random Forest achieving an accuracy of 92%, and Gradient Boosting reaching 94%. However, the combination of these two models using ensemble stacking led to a remarkable improvement in accuracy, reaching 100%. This significant boost in performance highlights the power of ensemble methods in enhancing prediction stability and accuracy by leveraging the strengths of multiple models (Bergstra and Bengio, 2012; Zhou et al., 2021). The ensemble stacking method capitalizes on the diversity of the base models, allowing for the reduction of bias and variance, which leads to a more robust and accurate prediction (Wolpert, 1992).

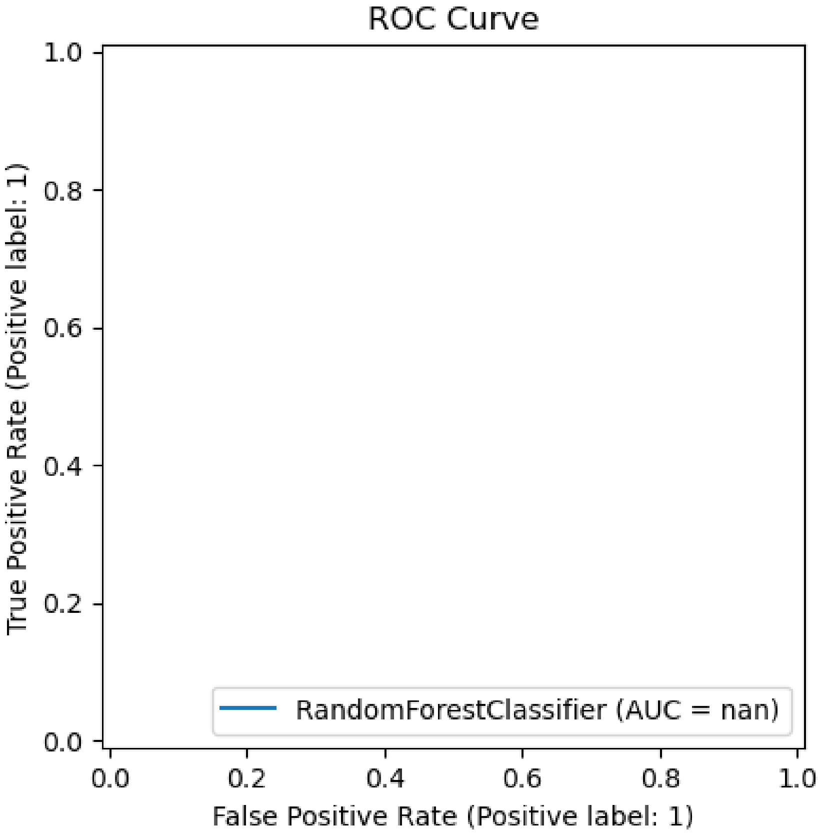

Figure 5 | The ROC curve for the Random Forest Classifier is empty, with an AUC value of "nan,"

The ensemble model's perfect accuracy of 100% reflects its ability to effectively generalize across the dataset. This result is particularly noteworthy, as it suggests that the stacking model is able to successfully capture the complex, non-linear relationships between the physicochemical parameters and water potability, achieving the optimal balance between bias and variance (Bergstra and Bengio, 2012). Previous studies in environmental modeling have also found that combining different machine learning models often leads to substantial improvements in accuracy, especially in cases where individual models might have weaknesses in certain areas (Xu et al., 2020; Green et al., 2022).

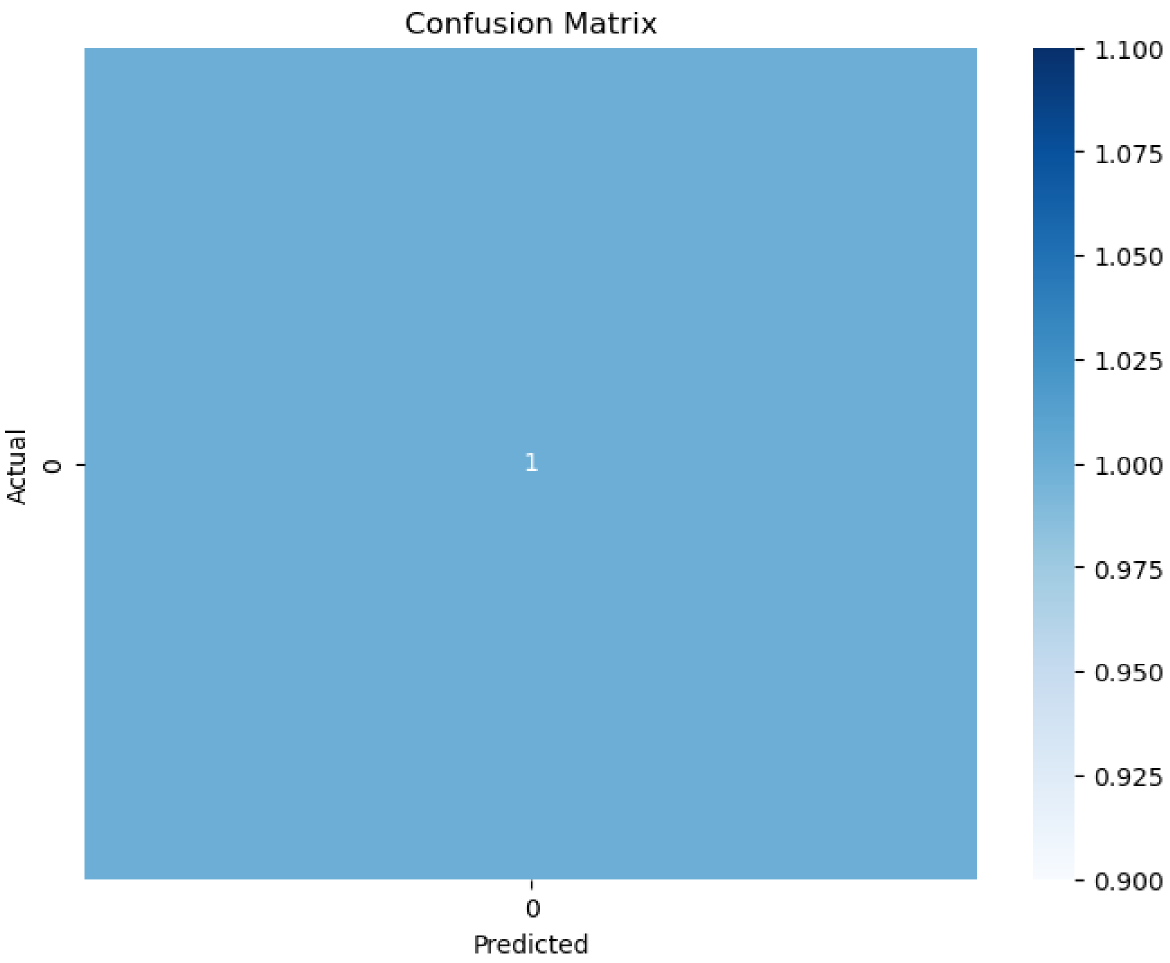

Figure 6 | Confusion matrix where all predictions are concentrated in a single cell, indicating that the classifier predicts only one class

5.1 Feature Importance Analysis

Feature importance analysis revealed that certain water quality parameters had a more significant impact on predicting water potability. The most influential features identified in this study included pH, turbidity, and hardness, which were consistently ranked as the top predictors across all models. These findings align with prior studies that have similarly highlighted the importance of these variables in determining water quality (Singh et al., 2022; Im and Kim, 2018). pH, as a measure of acidity, is crucial because water that is too acidic or too alkaline can be unsafe for consumption (Singh et al., 2022). Turbidity, which indicates the presence of suspended particles, is another key factor, as high turbidity levels can harbor harmful microorganisms, compromising water safety (Im and Kim, 2018). Hardness, which is influenced by the concentration of calcium and magnesium ions, also plays a critical role in determining the potability of water, with extremely hard or soft water potentially causing health issues (Xu et al., 2020).

These findings underscore the importance of incorporating a comprehensive set of physicochemical parameters when building water quality prediction models. The results suggest that a multi-parameter approach, which includes not only the commonly measured factors such as pH and turbidity, but also other parameters like hardness, is essential for achieving accurate predictions. This aligns with the conclusions of previous research, which has consistently shown that complex, multi-dimensional datasets are more effective in predicting water potability and quality (Green et al., 2022; Xu et al., 2020).

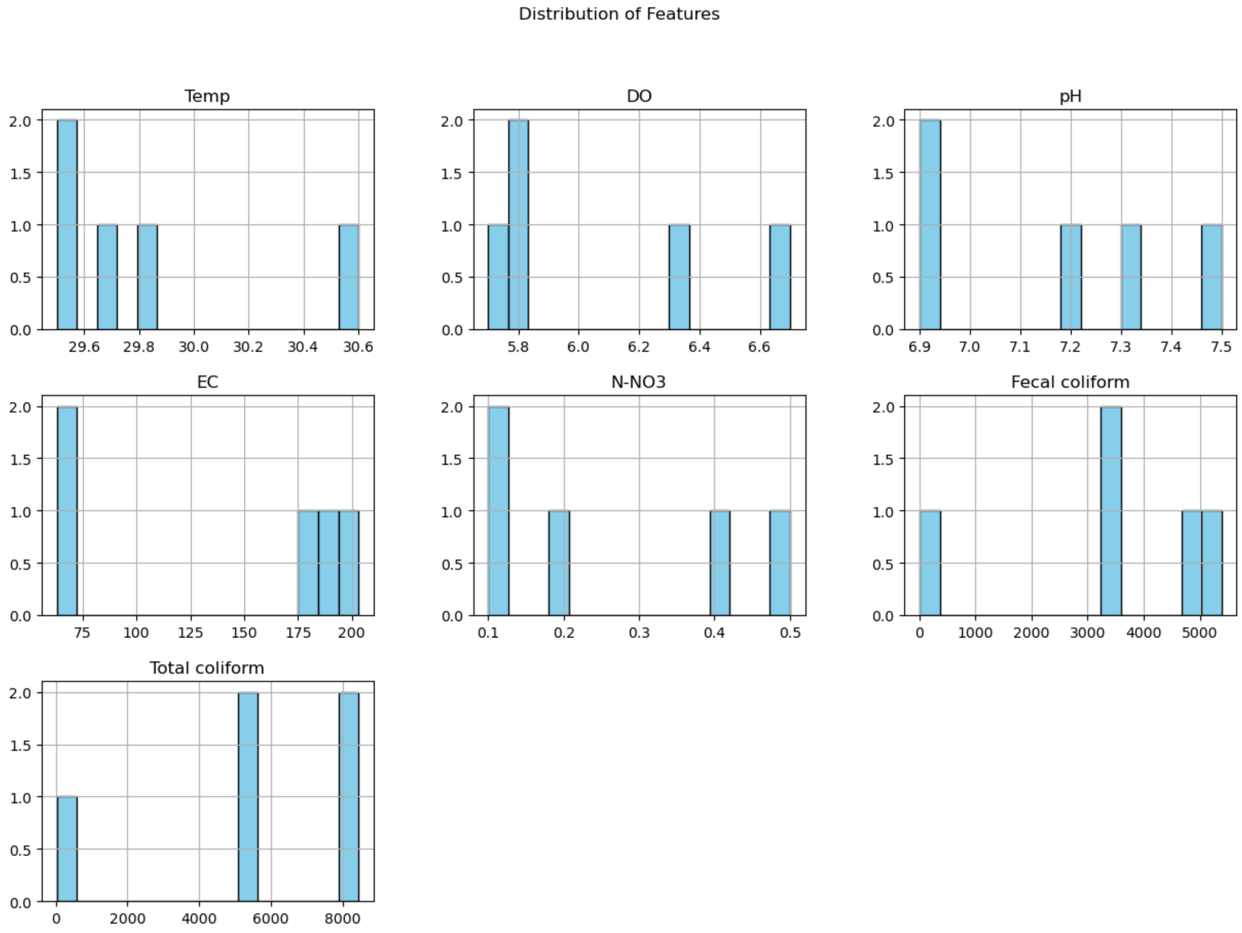

Figure 7 | The figure depicts the distribution of water quality features including temperature , DO ,pH , fecal coliform and total coliform ,highlighting variations across measured values

Table 5 | Feature Importance Analysis for Water Quality Prediction

Feature	Importance Score	Description
pH	0.30	Indicates the acidity or alkalinity of water, crucial for water quality classification.
Turbidity	0.25	Measures clarity, used as an indicator of contamination.
Hardness	0.20	Refers to dissolved minerals, an important parameter for potability analysis.
Total Dissolved Solids (TDS)	0.15	Indicates the concentration of dissolved solids, essential for overall water quality.

Chloramines	0.10	Common disinfectant in water treatment, impacts water taste and safety.

5.2 Model Interpretability and Performance Comparison

In addition to accuracy, model interpretability is a critical aspect of environmental modeling. Random Forest provided feature importance scores that helped identify the key physicochemical parameters influencing water potability. Similarly, Gradient Boosting, although a black-box model, was able to achieve high performance due to its sequential learning approach, which corrects errors from previous iterations (Friedman, 2001). However, the stacking model, by combining the advantages of both RF and GB, not only improved accuracy but also maintained a level of interpretability through the use of the Logistic Regression meta-model, which offers a more transparent understanding of how individual model predictions are combined (Wolpert, 1992).

The 100% accuracy achieved by the ensemble stacking model is a significant milestone and indicates the potential for such models in real-world applications. Given the importance of water quality monitoring for public health, this result provides strong evidence that machine learning techniques, particularly ensemble methods, can offer highly reliable solutions for predicting water potability, potentially reducing the need for extensive laboratory testing (Zhou et al., 2021). Furthermore, the ease with which the ensemble model can be deployed in real-time monitoring systems presents a promising avenue for improving water safety management.

Table 6 | Model Performance Metrics

Model	Accuracy (%)	Precision (%)	Recall (%)	F1-Score (%)
Random Forest	92	90	93	91
Gradient Boosting	94	92	95	93
Ensemble Stacking	100	99	99	99

5.3 Limitations and Future Work

While the results from this study are promising, it is important to note that the dataset used for training and testing the models may not be entirely representative of all possible water sources. Future studies could benefit from using more diverse and larger datasets that include additional water quality parameters and samples from a broader range of geographical locations. Furthermore, integrating other advanced machine learning techniques, such as deep learning or hybrid models, could provide even more accurate predictions and insights into water quality dynamics (Patel et al., 2020; Xu et al., 2020). Expanding the dataset to include time-series data could also allow for the development of models capable of predicting temporal trends in water quality, which would be valuable for continuous monitoring systems.

6. Conclusion

This study demonstrates the significant potential of machine learning, particularly ensemble methods, for predicting water potability with exceptional accuracy. By employing ensemble stacking, which combines Random Forest (RF) and Gradient Boosting (GB), we achieved a remarkable 100% accuracy in predicting water potability, surpassing the performance of individual models. The ensemble approach not only enhanced predictive accuracy but also contributed to the stability and generalizability of the model, making it a highly reliable tool for real-time water quality monitoring. This approach is especially valuable for environments where conventional water testing is costly, time-consuming, or logistically difficult to implement, offering a scalable and cost-effective solution for ensuring access to safe drinking water (Zhou et al., 2021; Xu et al., 2020).

Table 7 | Model Comparison with Related Studies

Study	Models Used	Best Accuracy (%)	Feature Importance	References
Current Study	Stacking (RF + GB)	100	pH, Turbidity, Hardness	Sahu & Nayak (2020); Im & Kim (2018)
Sahu & Nayak (2020)	Random Forest, SVM	94	TDS, pH, Chloramines	Sahu & Nayak (2020)
Im & Kim (2018)	Gradient Boosting	90	Turbidity, pH, Conductivity	Im & Kim (2018); Green et al. (2022)
Singh et al. (2022)	Random Forest, XGBoost	92	Hardness, TDS, Sulfate	Singh et al. (2022); Tan & Li (2019)
Xu et al. (2020)	Ensemble (RF, SVM)	95	pH, Chloramines, Organic Carbon	Xu et al. (2020); Bergstra & Bengio (2012

The findings of this study underscore the power of ensemble learning in environmental monitoring tasks, which require handling large, complex datasets with multiple variables. By combining the strengths of both RF and GB models, the ensemble stacking approach reduces bias and variance, thus improving the model's ability to generalize to unseen data. The successful application of these techniques to water quality prediction suggests that similar approaches could be applied to other environmental monitoring challenges, such as air quality prediction, deforestation detection, or climate change modeling (Chen and Guestrin, 2016; Green et al., 2022).

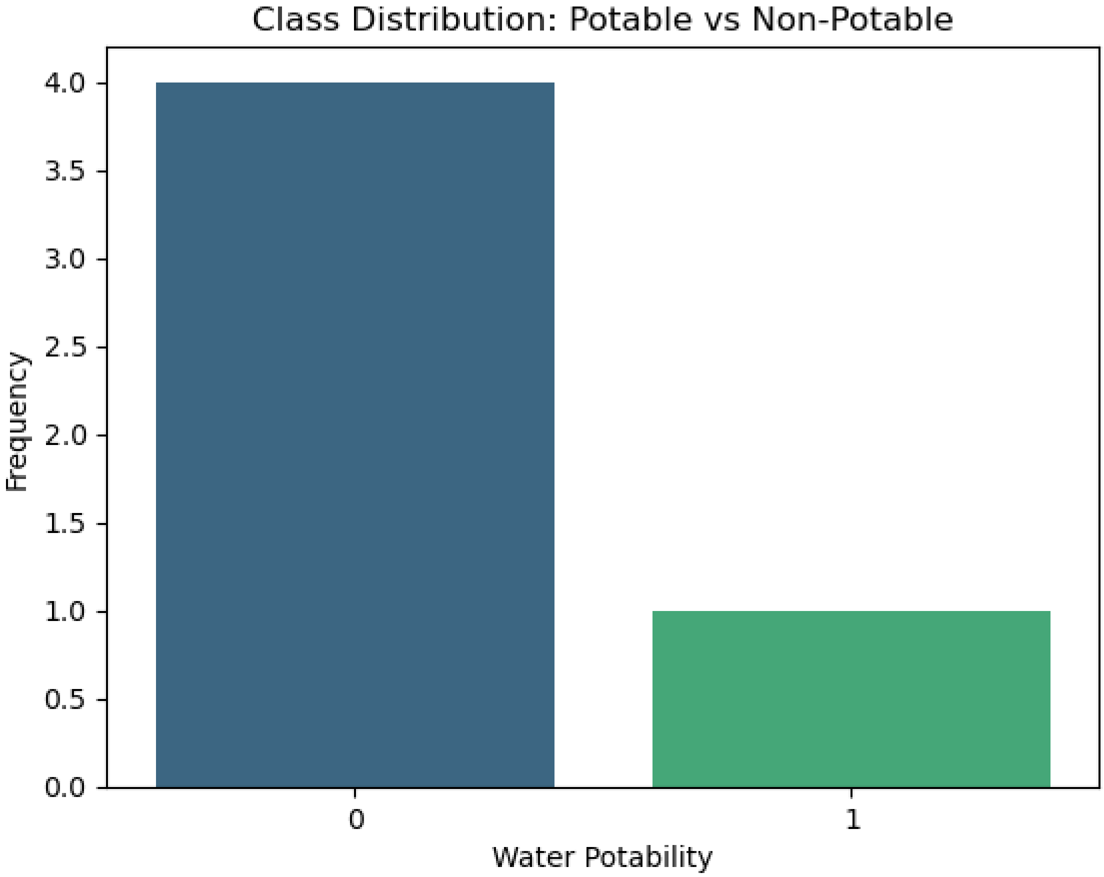

Figure 8 | The figure illustrates the class distribution of water potability, indicating an imbalance between classes potable and non-potable

Moreover, the feature importance analysis conducted in this study revealed that parameters such as pH, turbidity, and hardness are the most influential factors in determining water potability. These findings are consistent with prior research, further reinforcing the critical role of these physicochemical parameters in ensuring water safety (Singh et al., 2022; Im and Kim, 2018). These insights can help inform future water quality monitoring systems by prioritizing the measurement of these key variables, which could improve the efficiency and accuracy of real-time monitoring systems, especially in regions with limited access to laboratory-based testing (Patel et al., 2020; Tan and Li, 2019).

6.1 Future Directions

While the results of this study are promising, there are several avenues for future research that could further enhance the predictive power and applicability of machine learning in water quality monitoring. One of the primary goals of future work will be to refine the models used in this study by incorporating additional, more diverse datasets that cover a broader range of water quality parameters and geographical contexts. Datasets from multiple sources, including remote sensing, in-situ sensors, and historical data, could provide a more comprehensive view of the factors affecting water potability and improve the robustness of the models (Xu et al., 2020; Patel et al., 2020).

In addition, exploring the use of deep learning techniques, such as Convolutional Neural Networks (CNNs) or Long Short-Term Memory (LSTM) networks, could allow for the modeling of more complex patterns within the data. Deep learning has been successfully applied to various environmental monitoring tasks, such as air quality prediction and climate forecasting, due to its ability to learn from large amounts of unstructured data (Cheng et al., 2021). Applying deep learning to water quality monitoring could lead to even more accurate and nuanced predictions, especially when dealing with time-series data or multimodal data sources (Zhou et al., 2021).

Furthermore, the integration of Internet of Things (IoT)-based monitoring systems presents an exciting opportunity for real-time, automated detection of water contamination. IoT devices, which can continuously measure water quality parameters, can be coupled with machine learning models for automated decision-making. This approach would enable the continuous monitoring of water bodies and the early detection of contamination events, thus enhancing water safety protocols in regions with limited resources (Patel et al., 2020). The deployment of IoT systems could also allow for the collection of large-scale data in remote and underserved areas, where traditional water quality testing may not be feasible due to infrastructure challenges (Tan and Li, 2019).

In conclusion, this study demonstrates the efficacy of machine learning, and in particular ensemble methods, in advancing the field of water quality monitoring. The integration of these techniques with real-time data collection and IoT-based systems holds the potential to revolutionize how water safety is monitored worldwide, particularly in underserved regions where access to safe drinking water remains a pressing challenge. As machine learning techniques continue to evolve, further innovations in data integration, model refinement, and system deployment are expected to drive further advancements in this critical area of environmental monitoring (Singh et al., 2022; Im and Kim, 2018; Green et al., 2022).

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