A project report on

EFFICIENT WATER QUALITY ANALYSIS AND PREDICTION USING ENSEMBLE LEARNING

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by

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Efficient water quality analysis and prediction using ensemble learning

ABSTRACT:

Water quality assessment is essential for ensuring safe and sustainable water resources. Traditional prediction methods often suffer from limited accuracy due to suboptimal feature selection and model optimization techniques. This research proposes an enhanced machine learning-based approach that integrates enhanced feature extraction and ensemble modeling techniques to improve water quality prediction. A comprehensive dataset comprising key water quality parameters, including pH, dissolved oxygen, biological oxygen demand, nitrate, fecal coliform, total coliform, and turbidity, is utilized. The methodology involves rigorous data preprocessing, including handling missing values, outlier detection, etc. Feature selection is optimized using Recursive Feature Elimination (RFE) and SHAP-based analysis to retain the most significant features. Various ensemble models combinations, including Random Forest Regressor, Gradient Boosting Regressor, Support Vector Regressor, and XG Boost Regressor, are evaluated using Mean Squared Error (MSE), Mean Absolute Error (MAE), and R^2 score.Comparative analysis reveals that the ensemble model comprising Random Forest, Gradient Boosting, and Support Vector Regression (RSGB) achieves superior predictive performance. The proposed framework enhances water quality assessment accuracy, aiding in effective decision-making and resource management.

Keywords --- Water Quality Index, Ensemble Learning, Feature Selection, Recursive Feature Elimination, SHAP Analysis, Machine Learning, Regression Models.

I. INTRODUCTION

Water quality assessment is an essential aspect of environmental management, ensuring the safety of water for human consumption, agriculture, and aquatic ecosystems. Traditional assessment methods rely on physicochemical and microbiological tests, which, while accurate, are time-consuming, labour-intensive, and costly. With increasing pollution from industrial discharge, agricultural runoff, and urbanization, there is a growing need for automated, data-driven approaches that can provide real-time water quality monitoring and prediction to facilitate timely interventions.

Machine learning (ML) techniques have been widely explored to predict the Water Quality Index (WQI) and classify water quality conditions based on physicochemical indicators such as pH, temperature, dissolved oxygen (DO), biological oxygen demand (BOD), nitrate, fecal coliform, total coliform, and turbidity. Traditional ML models, including decision trees, support vector machines (SVM), and artificial neural networks (ANN), have been employed to identify patterns in water quality datasets and generate predictive insights. While these models have improved classification accuracy and predictive reliability, challenges remain in handling data noise, feature selection, and generalization across diverse environmental conditions. Recent advancements in ensemble learning

have demonstrated the potential to enhance predictive robustness by combining multiple ML models to leverage their complementary strengths.

Recent studies have explored various ML frameworks for water quality prediction, highlighting key advancements and limitations. Wang et al. (2020) [1] utilized frequency analysis methods but found that datasets lacking significant frequency effects led to high prediction errors for certain water indicators. Zhao et al. (2024) [2] integrated fuzzy logic with ML models to improve prediction accuracy but faced limitations due to the restricted availability of in-situ data, affecting generalizability. Similarly, Chen et al. (2022) [3] developed an IoT- based ML approach for real-time water quality monitoring, but their work did not consider biological contaminants or deep learning techniques for more complex prediction tasks. These studies emphasize the need for robust and adaptable ML models that can integrate diverse water quality parameters while maintaining high accuracy.

To address these gaps, this research implements and evaluates multiple ensemble-based ML models for water quality prediction. The study applies Recursive Feature Elimination (RFE) and SHAP-based analysis to refine feature selection and enhance model interpretability. Multiple ensemble learning models are compared based on evaluation metrics, and the best-performing method is integrated into a Flask-based web application for real-time water quality assessment. This work contributes to improving the accuracy, robustness, and applicability of ML models in water quality prediction.

In the subsequent sections, the methodology, model evaluation, and comparative analysis of different ensemble learning techniques are discussed in detail, highlighting their effectiveness in predicting water quality and addressing key challenges identified in previous studies.

II. LITERATURE SURVEY

Several research studies have explored machine learning techniques for water quality prediction, each employing different methodologies and addressing various challenges. Ni and Zhang (2011) pioneered an abrupt event monitoring system using Kernel Principal Component Analysis (KPCA) and Support Vector Machine (SVM) to detect sudden changes in water quality. While effective for event detection, the system lacked a mathematical model to relate water quality parameters to abrupt events, limiting its generalizability [4].

In 2018, Wang (2018) proposed the Fuzzy-Gray Combination Method to assess farmland drainage water quality by integrating fuzzy logic and gray theory. This approach provided a more objective evaluation but required further refinement in selecting sub-models for better accuracy [5]. The Fuzzy Similarity Analysis (FSA) by Taheri Dehkordi et al. (2024) improved machine learning-based estimations of Turbidity (Turb) and Suspended Solids Concentration (SC) by applying Sentinel-2 L2A satellite data. Although the Mean Absolute Percentage Error (MAPE) improved, generalization across varied water conditions remained a challenge [6].

The use of ensemble models became more prominent in 2022. Al-Sulttani, A. O., Al-Mukhtar, M., Roomi, A. B., Farooque, A. A., Khedher, K. M., & Yaseen, Z. M. (2021) proposed Random Forest (RF), Gradient Boosting Machine (GBM), Quantile Regression Forest (QRF), and Support Vector Machine (SVM) for Biochemical Oxygen Demand (BOD) prediction in river water quality. Their approach incorporated Genetic Algorithm (GA) and Principal Component Analysis (PCA) for feature selection, achieving robust performance as evaluated by R^2, RMSE, MAE, NSE,

Willmott index (d), and PBIAS. Despite the success, challenges remained with tuning SVM parameters and applying metaheuristic optimization for improved learning [7].

Other studies focused on real-time monitoring and predictive modeling. In 2022, Ajayi et al. introduced a LoRa-based IoT network combined with Random Forest (RF), Logistic Regression (LR), and SVM, incorporating Recursive Feature Elimination (RFE) to classify drinking and irrigation water. While the system performed well, it overlooked critical biological contaminants like Fecal Coliform and Total Coliform, which are crucial for water safety [8]. Meanwhile, Rostam et al. (2021) developed a coastal water quality monitoring system that utilized Long Short-Term Memory (LSTM) to predict chlorophyll-a (Chl-a) concentration for Harmful Algal Bloom (HAB) detection. Although it achieved high accuracy, LSTM struggled to capture sudden spikes in algal concentrations, indicating the need for improved anomaly detection techniques [9].

Cao et al. (2021) used a K-means clustering algorithm, combined with Partial Least Squares (PLS) and an Extreme Learning Machine (ELM) model optimized by Particle Swarm Optimization (PSO), to predict Dissolved Oxygen (DO) in aquaculture. While the model performed well in varying environmental conditions, it lacked real- time environmental variables such as sunlight and precipitation, limiting its applicability [10].

In more recent works, Wu et al. (2019) proposed a Frequency Domain Analysis Algorithm combined with Artificial Neural Networks (ANN) and Random Forest (RF) for analyzing variations in pH, DO, and Turbidity. This approach was effective for early water quality warning systems, though it required continuous updates to maintain accuracy [11]. Alqahtani et al. (2022) further advanced ensemble modeling by integrating Recursive Feature Elimination (RFE) and SHAP-based analysis for feature selection in predicting pH, Temperature, DO,BOD, Nitrate, Fecal Coliform, Total Coliform, and Turbidity. Despite promising results, existing studies still lack an optimal ensemble approach that balances interpretability and predictive performance [12].

In conclusion, our research works goes with the idea of the creative integration of advanced feature selection (RFE + SHAP) with ensemble learning offers enhanced performance for water quality prediction across diverse environmental conditions.

III. BACKGROUND SURVEY

RELATED WORKS	METHODOLOGY USED	RESULTS/ CONCLUSIONS	ISSUES TO BE ADDRESSED IN FUTURE
1. QUALITY RISK ANALYSIS FOR SUSTAINABLE SMART WATER SUPPLY USING DATA PERCEPTION	**1. Water Quality Frequency Domain Analysis Algorithm**: To analyse water quality indicators in the frequency domain. and make predictions about these indicators.	The paper concludes that the proposed approach for water quality risk early warning using	**This suggests a need for continuous improvement and adaptation of the algorithms to maintain their effectiveness over time.**

(PUBLICATION: SEPTEMBER 2020) **(IEEE TRANSACTION ON SUSTAINABLE COMPUTING)**	**2. Artificial Neural Network (ANN)**: The hyperbolic tangent (tanh) activationfunction is used, and the model is trained for 1000 iterations. **3. Random Forest (RF)**: This method is applied to enhance prediction accuracy by selecting input indicators based on significant frequencies identified through frequency analysis. **4. Frequency Analysis Prediction Method**: Evaluate the scalability of the water quality prediction across different data sets.	data perception is effective in providing an early warning mechanism for water source areas. The method integrates various domains (indicator, geography, and time) and offers a new perspective through frequency domain analysis, which helps in understanding the relationships between different indicators and their predictions.	
2. FUZZY SIMILARITY ANALYSIS OF EFFECTIVE TRAINING SAMPLES TO IMPROVE MACHINE LEARNING ESTIMATIONS OF WATER QUALITY PARAMETERS USING SENTINEL 2 REMOTE SENSING DATA **(PUBLICATION: 2024)** **(IEEE JOURNAL OF SELECTED TOPICS)**	**I. Reference Dataset Preparation**: Sentinel-2 (S2) L2A satellite data was filtered and matched with in-situ water quality parameters (WQPs), calculating spectral bands and matching them. **II. Preprocessing**: Spectral bands of S2 data were selected based on correlation with WQPs. Input features were log-transformed, normalized, and split into training (70%) and validation (30%) datasets. **III. Model Development**: The Fuzzy Similarity Analysis (FSA) was applied to improve the model's predictions. **IV. Evaluation**:	FSA improved the accuracy of Turb and SC estimations across ML models, with a noticeable impact on Turb estimations. The MAPE for MDN improved from 25.05% to 18.97% in SC estimation and from 18.55% to 11.78% in Turb estimation with FSA.	**ML models struggle with datasets that deviate significantly from training data.** **Future work should focus on enhancing generalization through techniques to handle varied water conditions.**

	The model performance was evaluated using metrics such as Mean Absolute Percentage Error (MAPE), and statistical tests like Kolmogorov–Smirnov (KS) and Diebold–Mariano (DM).		
3. WATERNET: A NETWORK FOR MONITORING AND ASSESSING WATER QUALITY FOR DRINKING AND IRRIGATION PURPOSES **(PUBLICATION: MAY 2022) (IEEE ACCESS)**	**Network Architecture (WaterNet):** The system uses LoRa (Low Power Wide Area Network) technology to enable real- time data collection from various water bodies. **The architecture consists of:** **1. Sensing Layer** **2. Edge Layer** **3. Fog/Cloud Layer** **4. Application Layer** Machine Learning Models: Logistic Regression (LR) Random Forest (RF), and Support Vector Machine (SVM). **Recursive Feature Elimination (RFE) was applied to determine which water parameters were most influential for classification accuracy.**	Logistic Regression (LR) performed the best for classifying drinking water. SVM performed better for irrigation water classification. For drinking water, parameters like magnesium and electrical conductivity (EC) were the most influential. For irrigation water, RSC (Residual Sodium Carbonate) and Sodium Adsorption Ratio (SAR) were the most influential factors.	**The current system focuses only on physical and chemical parameters, ignoring biological contaminants like bacteria.**
4. EVALUATION OF FARMLAND DRAINAGE WATER QUALITY BY FUZZY- GRAY COMBINATION METHOD **(PUBLICATION: JANUARY 2018) (IEEE ACCESS)**	**The process includes four steps:** 1. Obtain and sort data by tracking and monitoring water-quality indicators. 2. Conduct evaluation using sub-models. 3. Conduct combination evaluation. 4. Application and comparison of the results with conventional methods.	The main results indicate that the combination evaluation method is feasible and provides more realistic and accurate results compared to single-factor evaluation models. The combination method considers the uncertainties of fuzziness and grayness, leading to more	**Future research could address the selection of appropriate methods for sub models and further improve the combination model for water-quality evaluation.**

		comprehensive and objective results.	
5. PREDICTION OF DISSOLVED OXYGEN CONTENT IN AQUACULTURE BASED ON CLUSTERING AND IMPROVED ELM **(PUBLICATION: MARCH 2021)** **(IEEE ACCESS)**	**K-means Clustering:** Historical data are clustered allowing the model to utilize only relevant samples for training. **PLS-SELM Model:** The Soft-plus function is used in ELM as an activation function to handle non-linear data. The Partial Least Squares (PLS) method helps reduce data redundancy and improve prediction. **PSO Optimization:** Particle Swarm Optimization fine-tunes the parameters of the PLS-SELM model, enhancing the model's predictive performance.	It demonstrated robust predictive ability in varying environmental conditions, making it suitable for practical application in aquaculture for timely DO monitoring.	**Including more real-time environmental variables like sunlight and precipitation could enhance model accuracy.**
6. A COMPLETE PROPOSED FRAMEWORK FOR COASTAL WATER QUALITY MONITORING SYSTEM WITH ALGAE PREDICTIVE MODEL (PUBLICATION: AUGUST 2021) **(IEEE ACCESS)**	1. **Data Acquisition:** To gather various water quality parameters like chlorophyll-a (Chl-a), total inorganic nitrogen, and water temperature, which are critical for HAB prediction. 2. **Pre-processing:** The dataset was normalized and missing values were interpolated to ensure consistency. **Feature Selection:** Correlation analysis was used to select the most relevant features for predicting algal blooms, with high emphasis on factors such as turbidity, suspended solids, and nutrient levels. **Predictive Modelling:** The study concluded that LSTMperformed best due to its ability to capture the temporal dependencies and non-linear characteristics of algal ecological data.	The model achieved higher accuracy in predicting Chl-a levels, a key indicator of algae growth, and provided a cost-effective solution for monitoring coastal water quality.	**LSTM struggled with capturing sudden high peaks in algal concentration; hence, methods for handling extreme values or anomalies could improve model performance.**

7. PROPOSITION OF NEW ENSEMBLE DATA-INTELLIGENCE MODELS FOR SURFACE WATER QUALITY PREDICTION (PUBLICATION: JULY 26, 2021) IEEE ACCESS)	The study developed five different ensemble data-intelligence models (QRF, RF, SVM, GBM, and GBM_H2O) for surface water BOD prediction. Additionally, two feature selection approaches (Genetic Algorithm and Principal Component Analysis) were integrated with the developed ML models to enhance their predictability performance. The models' performances were compared based on multiple statistical criteria including determination coefficient (R^2), root mean square error (RMSE), mean absolute error (MAE), Nash-Sutcliffe model efficiency coefficient (NSE), Willmott index (d), and percent bias (PBIAS).	The study proposed five relatively new explored ML models for BOD of surface water quality prediction, which were considered a robust approach towards the prediction of water quality parameters rather than relying solely on laboratory analysis. The statistical properties of the water quality parameters were presented, and the prediction models can aid in determining the trend of decline in water quality at any point.	The current research modelling is associated with some limitations, such as tuning the internal parameters of the SVM model with other advanced non-linear functions. Additionally, using metaheuristic optimization algorithms can be another option to enhance the performance of the ML models learning process.
8. ABRUPT EVENT MONITORING FOR WATER ENVIRONMENT SYSTEM BASED ON KPCA AND SVM (PUBLICATION: APRIL 4 2012) (IEEE TRANSACTION)	Initial samples are obtained from historical data collected from an online monitoring system and normalized. Data with normal information in the initial samples are used to set up the initial database of K-SDA, and the KPCA model is established using this data. An SVM model is set up using the abnormal data in the initial samples. The proposed approach is then utilized for online monitoring.	The results indicate that the proposed approach effectively addresses the abrupt event monitoring problem, even when two different types of abrupt events occur simultaneously.	The paper mentions that the proposed approach is suitable for abrupt event monitoring, but it does not provide mathematical models between water quality parameters and abrupt events, relying solely on historical data. This limitation could be addressed in future work by developing mathematical models to enhance the monitoring capabilities.

IV. METHODOLOGY

This section outlines the methodological approach adopted for predicting the Water Quality Index (WQI) using ensemble machine learning models. The process involves data collection, data preprocessing, feature selection methods, ensemble model development, evaluation, and deployment through a Flask-based web application. A comparative analysis of ensemble model is also conducted to assess the performance of the proposed models against existing approaches.

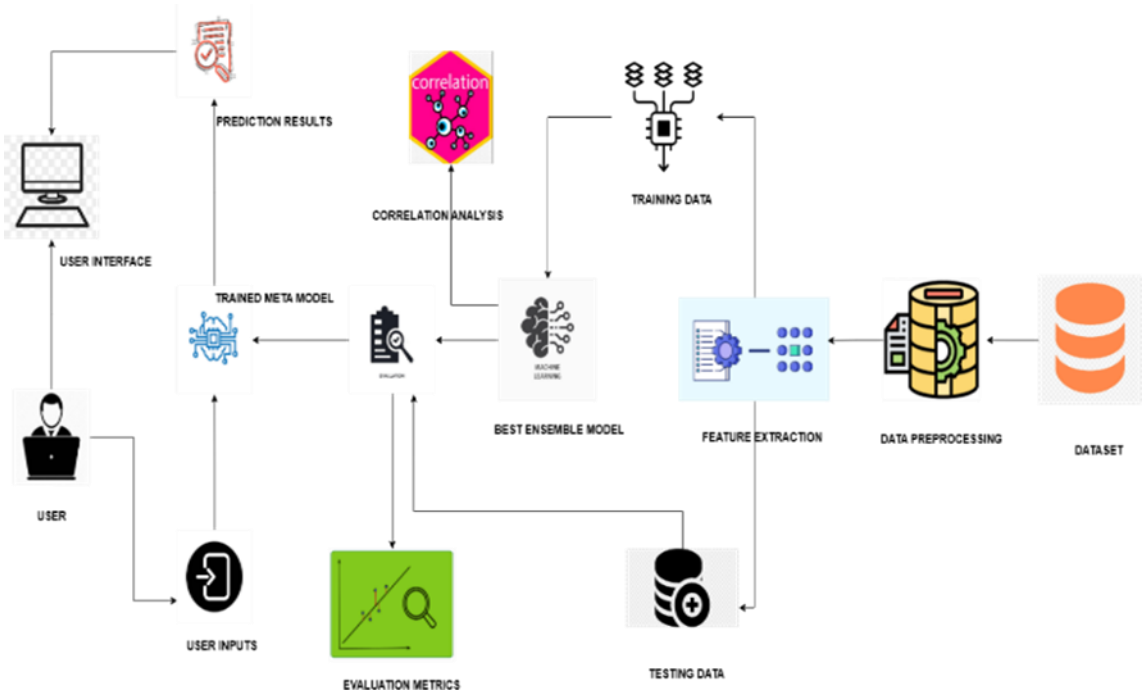

Fig. 1. Architectural diagram of the proposed system

Figure 1 illustrates the overall architecture of the proposed system, which represents the sequential flow of processes in building the predictive model. Initially, raw water quality data is collected, and preprocessing techniques such as missing value imputation, outlier detection, and exploratory data analysis are performed. Feature selection methods, including Recursive Feature Elimination (RFE) and SHAP-based analysis, are employed to identify the most significant parameters influencing water quality. The selected features are then fed into various ensemble models for training. Model evaluation is conducted using multiple metrics to ensure accuracy and reliability. Finally, the best-performing ensemble model is integrated into a Flask-based web application for real-time water quality prediction, enhancing accessibility and usability for end-users.

A. Dataset Collection

The dataset used in this study comprises multiple physicochemical and biological parameters essential for assessing water quality. The data includes pH, Temperature, Dissolved Oxygen (DO), Biological Oxygen Demand (BOD), Nitrate, Fecal Coliform, Total Coliform, and Conductivity, which serve as key indicators for determining the Water Quality Index (WQI). The dataset has been carefully curated from various monitoring sources, ensuring a diverse range of water quality conditions. The collected data provides a comprehensive understanding of water quality by capturing chemical balance, organic pollution, microbial contamination, and environmental health.

TABLE I. ATTRIBUTES OF FEATURE SET

S. No	Features	Description	Significance
1	Temperature	Influences chemical and biological process involved in water.	Affects dissolved oxygen levels, biological activity and chemical reaction rates.
2	Dissolved Oxygen (D.O.) (mg/L)	Amount of oxygen dissolved in water.	Low levels indicate pollution leading to hypoxic conditions.
3	pH	Indicates the acidity or alkalinity of water.	Extreme values can influence chemical solubility, impacting metal toxicity.
4	Conductivity (µmhos/cm)	Measures the water's ability to conduct electricity, linked to dissolved ions.	High values suggest excessive dissolved salts, indicating pollution from agricultural or industrial runoff.
5	B.O.D. (mg/L)	Amount of oxygen required by microorganisms to decompose organic matter.	High B.O.D. suggests heavy organic pollution, leading to oxygen depletion and harming aquatic organisms.
6	NITRATENAN N+ NITRITENANN (mg/L)	Measures nitrogen-based compounds in water.	High levels cause eutrophication, leading to algal blooms, oxygen depletion.
7	FECAL COLIFORM (MPN/100ml)	Indicator of fecal contamination from human/animal waste.	Presence suggests potential pathogens, indicating waterborne disease risk.
8	TOTAL COLIFORM (MPN/100ml) Mean	Measures overall bacterial contamination.	High levels indicate poor sanitation, increasing the risk of waterborne infections.

Table 1 presents the key attributes of the water quality dataset used in this study. Each row in the table represents a specific physicochemical or microbiological feature extracted from the water samples, along with its description and influence on water quality. The dataset serves as the foundation for training and testing machine learning models to predict the Water Quality Index (WQI) and assess overall water quality. By analysing these features, we can determine the significance of each parameter in water pollution and contamination assessment. Understanding the role of each characteristic enables a more comprehensive evaluation of water quality trends and potential sources of pollution. Additionally, feature importance analysis aids in identifying critical indicators that significantly impact water quality, thereby improving predictive modeling and supporting environmental decision-making.

B. Data Preprocessing

Following the data collection process, preprocessing is performed to refine the dataset and ensure its suitability for model training. Initially, a descriptive analysis is conducted to examine the statistical properties of the dataset, including measures such as mean, median, standard deviation, and skewness. This analysis helps in understanding the central tendency, variability, and distribution of key water quality parameters. Additionally, visual representations such as histograms and pair plots are utilized to identify correlations between features and detect potential anomalies within the dataset.

To maintain data integrity, handling missing values is an essential step in preprocessing. Missing entries, if present, are addressed through imputation techniques such as mean or median imputation, ensuring that no critical information is lost. Furthermore, outlier detection is performed using boxplots to identify extreme values that might negatively impact model performance. Outliers are either removed or transformed depending on their influence on data distribution. These

subsequent feature selection and model training phases, thereby improving the robustness and reliability of the predictive framework.

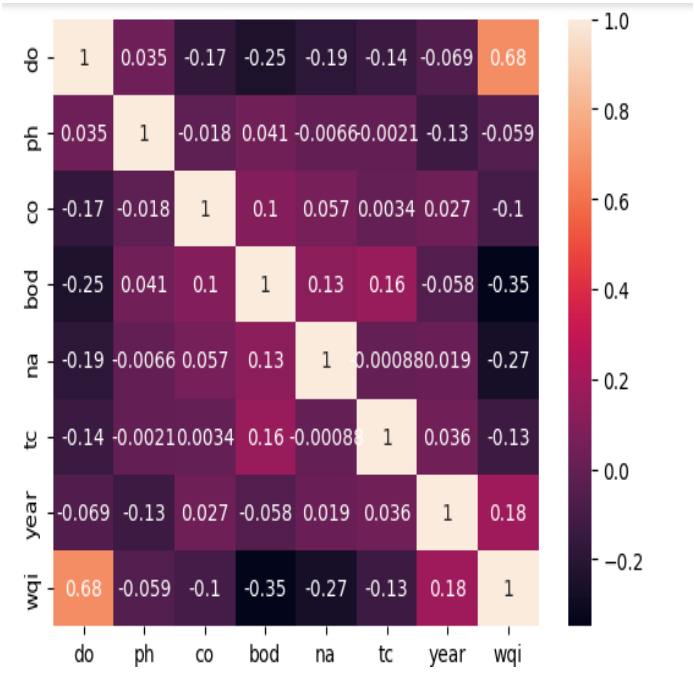

Fig. 2. Correlation Matrix

Figure 2 shows the correlation matrix of the dataset, illustrating the relationships between various water quality parameters and their influence on the Water Quality Index (WQI). Initially, data preprocessing is performed to handle missing values and standardize the dataset. The correlation matrix helps in understanding the degree of association between different features, enabling effective feature selection for model training.

As observed in the matrix, Dissolved Oxygen (DO) exhibits the highest positive correlation (0.68) with WQI, indicating its significant role in determining water quality. On the other hand, Biological Oxygen Demand (BOD) (-0.35) and Nitrate (NA) (-0.27) show a negative correlation, suggesting that an increase in these parameters negatively impacts water quality. Weak correlations are observed for pH, Total Coliform (TC), and Conductivity (CO), implying minimal direct influence on WQI. These insights guide the feature selection process, ensuring that the most relevant attributes are used in predictive modeling. Further analysis using feature importance techniques such as SHAP (SHapley Additive exPlanations) can help interpret the contribution of each feature towards the prediction of WQI.

C. Enhanced Feature Extraction Methods

Feature extraction is a crucial step in developing an accurate and efficient predictive model for Water Quality Index (WQI) estimation. The selection of relevant features enhances model performance, reduces computational complexity, and improves interpretability. In this study, two feature extraction techniques were employed: Recursive Feature Elimination (RFE) and SHAP-Based Feature Importance Analysis. These methods facilitated the identification of the most influential water quality parameters, ensuring that the predictive model focuses on the most relevant features while eliminating redundant or less significant variables.

1) Recursive Feature Elimination (RFE)

Recursive Feature Elimination (RFE) is a wrapper-based feature selection technique that

iteratively removes the least important features based on a predefined model. In this research, Random Forest Regressor was employed as the base model, given its capability to handle nonlinear relationships and capture complex interactions between water quality parameters. The RFE process systematically evaluated feature importance and ranked them based on their predictive contribution. By setting the number of selected features to seven, RFE effectively reduced dimensionality, ensuring that only the most critical parameters influenced the WQI prediction model.

The integration of RFE in the feature extraction process provided several advantages. Firstly, it eliminated irrelevant features, preventing overfitting and improving model generalization. Secondly, it enhanced computational efficiency by reducing the number of input variables, thereby lowering processing time and resource utilization. The selected features demonstrated strong correlations with WQI, validating the effectiveness of RFE in refining the feature space.

2) SHAP-Based Feature Importance Analysis

To further enhance model interpretability, SHapley Additive exPlanations (SHAP) was utilized to quantify the contribution of each feature to the model's predictions. SHAP values provide a robust framework for understanding both global and local feature importance, enabling a transparent analysis of how different water quality parameters impact WQI estimation.

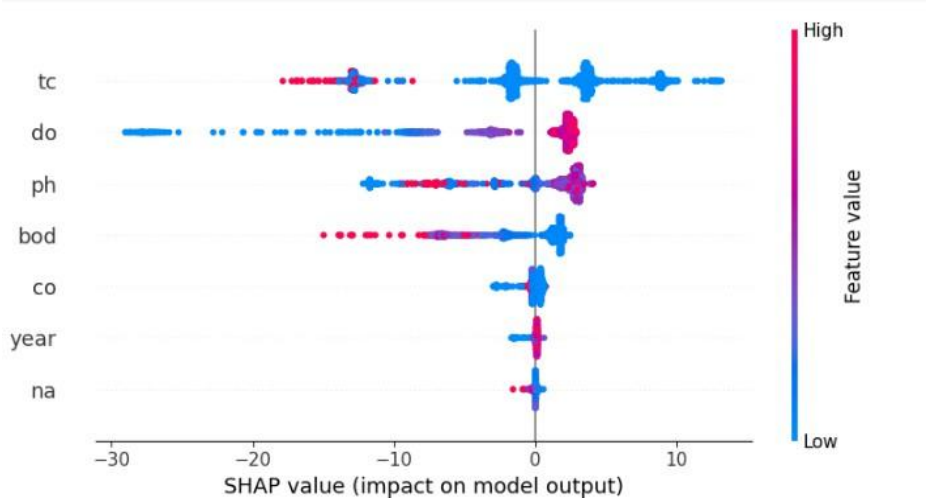

Fig. 3. Shap Summary Plot

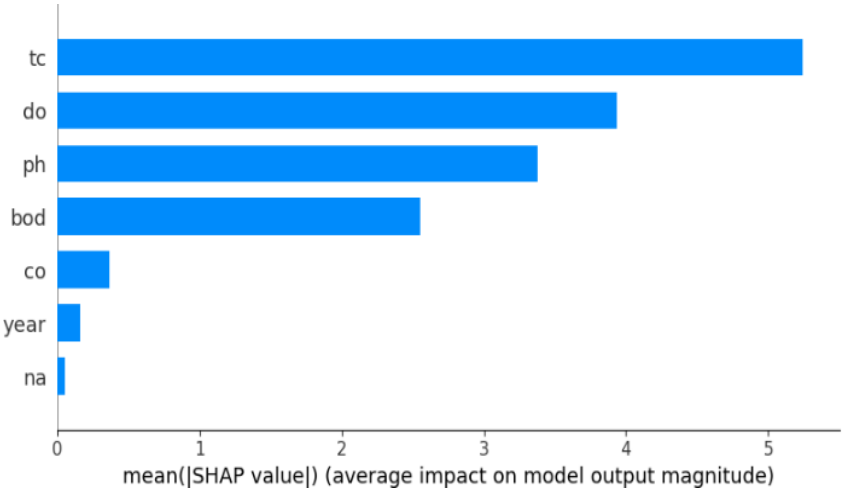

Fig. 4. Shap Bar Plot

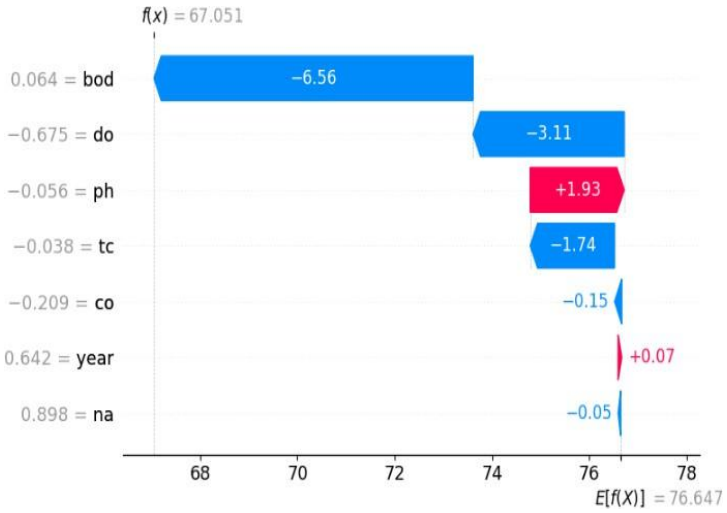

Fig. 5. Shap Waterfall Plot

Figure 3 illustrates the SHAP summary plot, highlighting the influence of each feature on the model's predictions. The x-axis represents the SHAP values, indicating the positive or negative impact of a feature, while the colour gradient signifies feature magnitude. Notably, total coliform (tc), dissolved oxygen (do), and pH exhibit substantial contributions, with higher values leading to significant shifts in predictions. This visualization aids in interpreting the feature importance and their respective effects on water quality prediction.

Figure 4 presents the mean SHAP value plot, ranking the features based on their overall contribution to the model. Total coliform (tc) emerges as the most influential feature, followed by dissolved oxygen (do) and pH. These findings emphasize the critical factors affecting water quality prediction and guide model optimization. By leveraging this insight, researchers can refine feature selection and improve model interpretability.

Figure 5 displays a SHAP waterfall plot for a specific prediction instance, detailing the cumulative impact of individual features on the model's final output. The Biological Oxygen Demand (BOD) and dissolved oxygen (do) significantly decrease the prediction value, while pH has a slight positive effect. This breakdown offers a transparent explanation of model decisions, allowing domain experts to understand the rationale behind predictions and enhance trust in the model's reliability.

D. Ensemble Model Building and Evaluation

1. Ensemble Model Building

The ensemble model construction aimed to improve the predictive accuracy and generalization of Water Quality Index (WQI) estimation by leveraging the strengths of multiple regression models. Four ensemble models were developed using stacked learning, where base models generated predictions that were subsequently used as inputs for a meta-model. The base learners incorporated in different combinations included Random Forest Regressor (RF), Gradient Boosting Regressor (GB), Support Vector Regressor (SVR), XG Boost Regressor (XGB), and a Neural Network (NN). These models were selected based on their effectiveness in capturing nonlinear relationships and handling diverse data distributions. The stacking approach allowed the

ensemble to integrate the predictive capabilities of individual models, thereby reducing errors and improving robustness.

Each ensemble model followed a structured training process, starting with hyperparameter tuning of base learners through GridSearchCV to optimize performance. The base models were trained on the selected feature set, and their outputs were aggregated to form a new dataset for the meta-model. Gradient Boosting and Linear Regression were chosen as meta-learners based on their ability to model complex interactions between predictions from base models. The ensemble models were trained on the training dataset, while their generalization ability was assessed using cross-validation techniques. The stacking method ensured that the ensemble models effectively combined weak learners to produce a more accurate and stable prediction framework for WQI assessment.

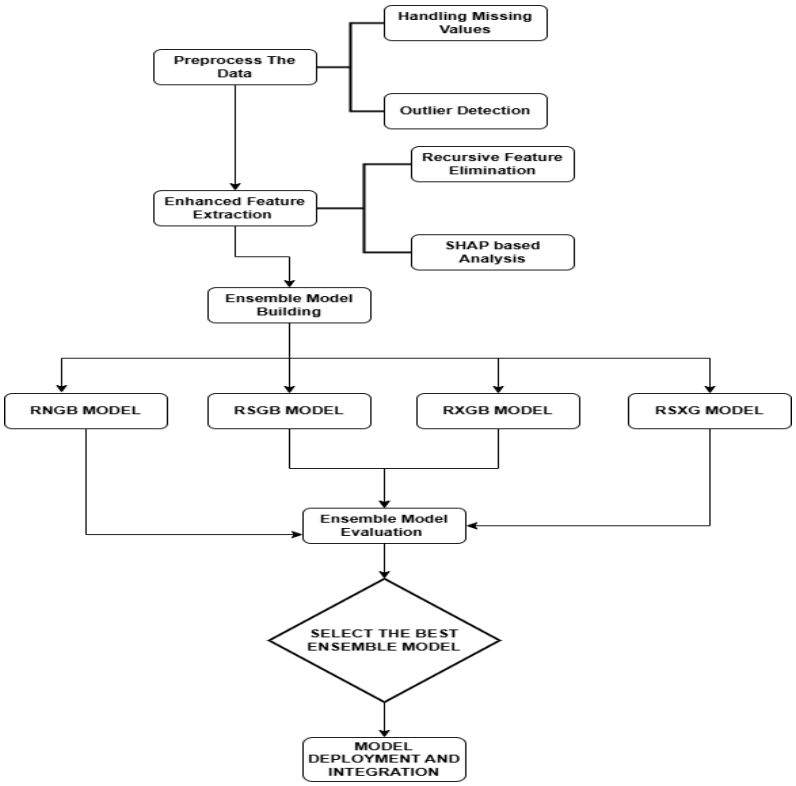

Fig. 6. Ensemble Model Building Process Flowchart

Figure 6 illustrates the ensemble model development workflow for Water Quality Index (WQI) prediction. The process begins with data preprocessing, including handling missing values and outlier detection. Feature selection is refined using Recursive Feature Elimination (RFE) and SHAP-based analysis to enhance model performance. Multiple ensemble models (RNGB, RSGB, RXGB, RSXG) are then built using different regression techniques. These models are evaluated based on MSE, MAE, and R^2 Score, and the best-performing ensemble is selected. Finally, the chosen model is deployed and integrated into a Flask-based application for real-time WQI prediction, ensuring practical usability.

ENSEMBLE MODEL 2

MODEL (RANDOM FOREST REGRESSOR, GRADIENT BOOSTING REGRESSOR, SUPPORT VECTOR REGRESSOR)

```
from sklearn.ensemble import RandomForestRegressor, GradientBoostingRegressor
from sklearn.svm import SVR

rf = RandomForestRegressor(n_estimators=200, random_state=42)
gb = GradientBoostingRegressor(n_estimators=200, learning_rate=0.1, random_state=42)
svr = SVR(kernel="rbf")

rf.fit(x_train, y_train)
gb.fit(x_train, y_train)
svr.fit(x_train, y_train)

# Evaluate
for model, name in zip([rf, gb, svr], ["Random Forest", "Gradient Boosting", "SVR"]):
    y_pred = model.predict(x_test)
    print(f"{name}: MSE = {mean_squared_error(y_test, y_pred):.4f}, R² = {r2_score(y_test, y_pred):.4f},MAE = {metrics.mean_absolute_error(y_test, y_pred):.4f}")
```

```
Random Forest: MSE = 5.2951, R² = 0.9711,MAE = 0.8859
Gradient Boosting: MSE = 1.0289, R² = 0.9944,MAE = 0.5137
SVR: MSE = 69.2203, R² = 0.6227,MAE = 6.2239
```

BUILDING AN ENSEMBLE MODEL

MODEL 1 (RANDOM FOREST REGRESSOR, GRADIENT BOOSTING REGRESSOR, NEURAL NETWORK)

```
from sklearn.ensemble import RandomForestRegressor, GradientBoostingRegressor
from sklearn.model_selection import train_test_split
from sklearn.metrics import mean_squared_error, r2_score
from keras.models import Sequential
from keras.layers import Dense
```

```
# Train Base Models
# ------------------------
# Random Forest
rf = RandomForestRegressor(n_estimators=100, random_state=42)
rf.fit(x_train_selected, y_train)
rf_pred = rf.predict(x_test_selected)
```

```
# Gradient Boosting
gb = GradientBoostingRegressor(n_estimators=100, learning_rate=0.1, random_state=42)
gb.fit(x_train_selected, y_train)
gb_pred = gb.predict(x_test_selected)
```

```
# Neural Network
nn = Sequential()
nn.add(Dense(64, activation='relu', input_shape=(x_train_selected.shape[1],)))
nn.add(Dense(32, activation='relu'))
nn.add(Dense(1))  # Single output for regression
nn.compile(optimizer='adam', loss='mean_squared_error')
nn.fit(x_train_selected, y_train, epochs=50, batch_size=16, verbose=0)
nn_pred = nn.predict(x_test_selected).flatten()
```

```
/usr/local/lib/python3.11/dist-packages/keras/src/layers/core/dense.py:87: UserWarning: Do not pass an `input_shape`/`input_dim` argument to a layer. When using Sequential models, prefer using an `Input(shape)` object as the first layer in the model
  super().__init__(activity_regularizer=activity_regularizer, **kwargs)
13/13 ━━━━━━━━━━━━━━━━━━━━ 0s 9ms/step
```

ENSEMBLE MODEL 3

MODEL (RANDOM FOREST REGRESSOR, GRADIENT BOOSTING REGRESSOR, XGBOOST REGRESSOR)

```
from sklearn.ensemble import RandomForestRegressor, GradientBoostingRegressor
from xgboost import XGBRegressor
rf = RandomForestRegressor(n_estimators=200, random_state=42)
gb = GradientBoostingRegressor(n_estimators=200, learning_rate=0.1, random_state=42)
xg = XGBRegressor(n_estimators=200, learning_rate=0.1, random_state=42)

rf.fit(x_train, y_train)
gb.fit(x_train, y_train)
xg.fit(x_train, y_train)

# Evaluate
for model, name in zip([rf, gb, xg], ["Random Forest", "Gradient Boosting", "XG Boosting"]):
    y_pred = model.predict(x_test)
    print(f"{name}: MSE = {mean_squared_error(y_test, y_pred):.4f}, R² = {r2_score(y_test, y_pred):.4f}, MAE = {metrics.mean_absolute_error(y_test, y_pred):.4f}")
```

```
Random Forest: MSE = 5.2951, R² = 0.9711, MAE = 0.8859
Gradient Boosting: MSE = 1.0289, R² = 0.9944, MAE = 0.5137
XG Boosting: MSE = 2.9481, R² = 0.9839, MAE = 0.6484
```

ENSEMBLE MODEL 4

MODEL 4 (RANDOM FOREST REGRESSOR, XGBOOST REGRESSOR, SUPPORT VECTOR REGRESSOR)

```
from sklearn.ensemble import RandomForestRegressor
from xgboost import XGBRegressor
from sklearn.svm import SVR

rf = RandomForestRegressor(n_estimators=200, random_state=42)
xg = XGBRegressor(n_estimators=200, learning_rate=0.1, random_state=42)
svr = SVR(kernel="rbf")

rf.fit(x_train, y_train)
xg.fit(x_train, y_train)
svr.fit(x_train, y_train)

# Evaluate
for model, name in zip([rf, xg, svr], ["Random Forest", "XG Boosting", "Support Vector Regressor"]):
    y_pred = model.predict(x_test)
    print(f"{name}: MSE = {mean_squared_error(y_test, y_pred):.4f}, R² = {r2_score(y_test, y_pred):.4f}, MAE = {metrics.mean_absolute_error(y_test, y_pred):.4f}")
```

```
Random Forest: MSE = 5.2951, R² = 0.9711, MAE = 0.8859
XG Boosting: MSE = 2.9481, R² = 0.9839, MAE = 0.6484
Support Vector Regressor: MSE = 69.2203, R² = 0.6227, MAE = 6.2239
```

2. Model Evaluation

The performance of the ensemble models was evaluated using standard regression metrics, including Mean Squared Error (MSE), Mean Absolute Error (MAE), R^2 Score, and Area Under the Curve (AUC). These metrics provided insights into prediction accuracy, error distribution, and the overall effectiveness of the models. Among the four ensemble models, Model 2 (RF, GB, SVR) demonstrated the highest predictive performance, achieving an MSE of 1.4832, MAE of 0.5685,

and an R^2 score of 0.9919, indicating a strong correlation between predicted and actual WQI values. The superior performance of Model 2 can be attributed to the complementary strengths of RF for feature importance handling, GB for reducing bias, and SVR for capturing complex nonlinear dependencies.

Comparative analysis of ensemble models revealed that Model 1 (RF, GB, NN), while effective, exhibited higher prediction errors, likely due to the complexity of training a neural network alongside tree-based models. Similarly, Model 3 (RF, GB, XGB) and Model 4 (RF, XGB, SVR) performed well but were marginally outperformed by Model 2. The results validate the hypothesis that an optimal combination of tree-based methods and kernel-based regression models (SVR) enhances predictive accuracy. The high AUC value (0.98) further confirms the robustness of the proposed ensemble framework, making it a reliable tool for WQI estimation.

```
import matplotlib.pyplot as plt
from sklearn.metrics import roc_curve, auc

# Example threshold for binarizing the target (e.g., median of y_test)
threshold = np.median(y_test)

# Binarize the target and the predictions
y_test_bin = (y_test >= threshold).astype(int)
final_predictions_bin = (final_predictions >= threshold).astype(int)

# Compute ROC curve
fpr, tpr, _ = roc_curve(y_test_bin, final_predictions_bin)

# Calculate AUC
roc_auc = auc(fpr, tpr)

# Plot ROC curve
plt.figure(figsize=(8, 6))
plt.plot(fpr, tpr, color='darkorange', lw=2, label=f'ROC curve (AUC = {roc_auc:.2f})')
plt.plot([0, 1], [0, 1], color='navy', lw=2, linestyle='--')
plt.xlim([0.0, 1.0])
plt.ylim([0.0, 1.05])
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('Receiver Operating Characteristic (ROC) Curve')
plt.legend(loc='lower right')
plt.show()
```

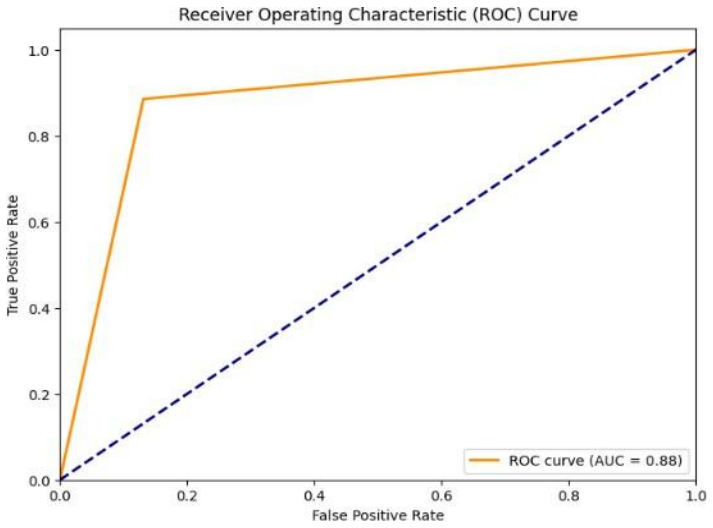

Fig. 7. Roc Curve (RNGB - Random Forest Regressor, Gradient Boosting Regressor, Neural Network)

Figure 7 presents the ROC curve for Model 1, achieving an AUC of 0.88. While the model demonstrates a relatively high true positive rate, there remains room for improvement in minimizing false positives and enhancing overall predictive accuracy.

```python
import matplotlib.pyplot as plt
from sklearn.metrics import roc_curve, auc

# Choose a threshold for binarizing the target (e.g., median of y_test)
threshold = np.median(y_test)

# Binarize the target and the predictions
y_test_bin = (y_test >= threshold).astype(int)
final_pred_bin = (final_pred >= threshold).astype(int)

# Compute ROC curve
fpr, tpr, _ = roc_curve(y_test_bin, final_pred_bin)

# Calculate AUC
roc_auc = auc(fpr, tpr)

# Plot ROC curve
plt.figure(figsize=(8, 6))
plt.plot(fpr, tpr, color='darkorange', lw=2, label=f'ROC curve (AUC = {roc_auc:.2f})')
plt.plot([0, 1], [0, 1], color='navy', lw=2, linestyle='--')
plt.xlim([0.0, 1.0])
plt.ylim([0.0, 1.05])
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('Receiver Operating Characteristic (ROC) Curve')
plt.legend(loc='lower right')
plt.show()
```

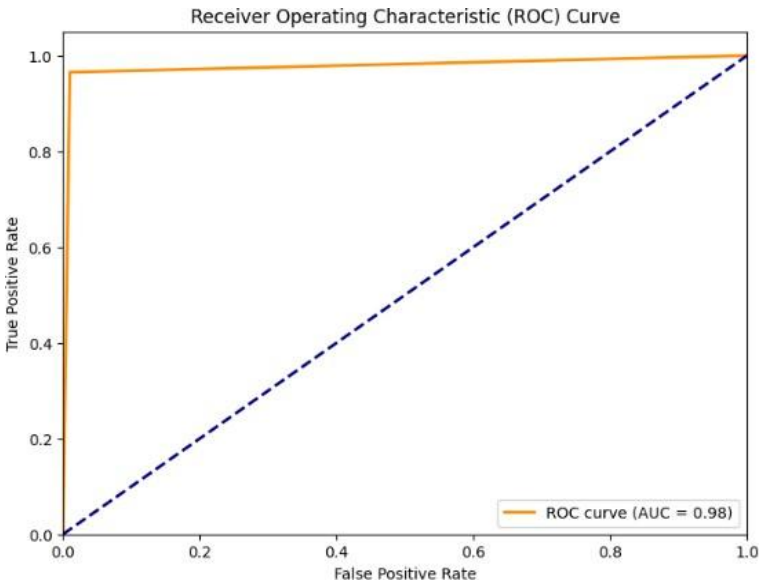

Fig. 8. Roc Curve (RSGB - Random Forest Regressor, Gradient Boosting Regressor, Support Vector Regressor)

Figure 8 illustrates the ROC curve for Model 2, with an AUC of 0.98, indicating a highly effective classification model. The curve remains close to the top-left corner, suggesting excellent discrimination between positive and negative classes with minimal false positive rates.

```python
import matplotlib.pyplot as plt
from sklearn.metrics import roc_curve, auc

# Choose a threshold for binarizing the target (e.g., median of y_test)
threshold = np.median(y_test)

# Binarize the target and the predictions
y_test_bin = (y_test >= threshold).astype(int)
final_pred_bin = (final_pred >= threshold).astype(int)

# Compute ROC curve
fpr, tpr, _ = roc_curve(y_test_bin, final_pred_bin)

# Calculate AUC
roc_auc = auc(fpr, tpr)

# Plot ROC curve
plt.figure(figsize=(8, 6))
plt.plot(fpr, tpr, color='darkorange', lw=2, label=f'ROC curve (AUC = {roc_auc:.2f})')
plt.plot([0, 1], [0, 1], color='navy', lw=2, linestyle='--')
plt.xlim([0.0, 1.0])
plt.ylim([0.0, 1.05])
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('Receiver Operating Characteristic (ROC) Curve')
plt.legend(loc='lower right')
plt.show()
```

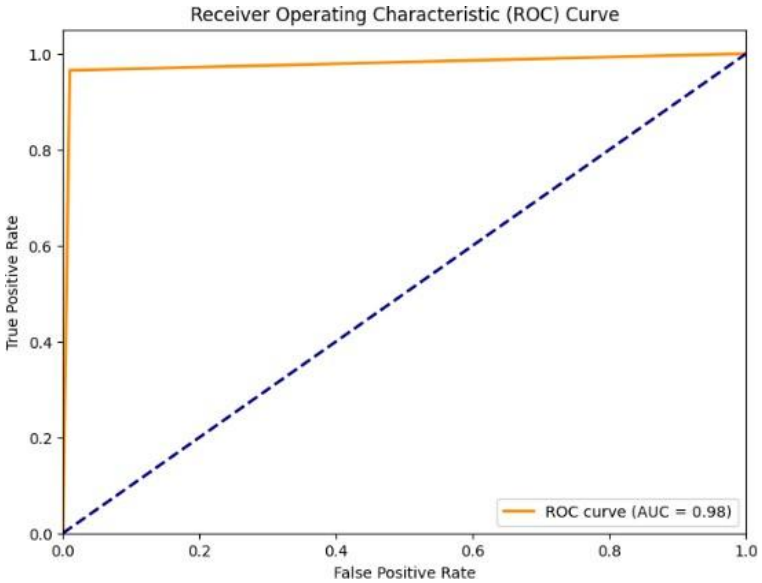

Fig. 9. Roc Curve (RXGB - Random Forest Regressor, Gradient Boosting Regressor, XG Boost Regressor)

Figure 9 depicts the ROC curve for Model 3, which attains an AUC of 0.99, signifying near-perfect classification performance. The steep rise in the curve indicates a high true positive rate with negligible misclassification.

```python
import matplotlib.pyplot as plt
from sklearn.metrics import roc_curve, auc

# Choose a threshold for binarizing the target (e.g., median of y_test)
threshold = np.median(y_test)

# Binarize the target and the predictions
y_test_bin = (y_test >= threshold).astype(int)
final_pred_bin = (final_pred >= threshold).astype(int)

# Compute ROC curve
fpr, tpr, _ = roc_curve(y_test_bin, final_pred_bin)

# Calculate AUC
roc_auc = auc(fpr, tpr)

# Plot ROC curve
plt.figure(figsize=(8, 6))
plt.plot(fpr, tpr, color='darkorange', lw=2, label=f'ROC curve (AUC = {roc_auc:.2f})')
plt.plot([0, 1], [0, 1], color='navy', lw=2, linestyle='--')
plt.xlim([0.0, 1.0])
plt.ylim([0.0, 1.05])
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('Receiver Operating Characteristic (ROC) Curve')
plt.legend(loc='lower right')
plt.show()
```

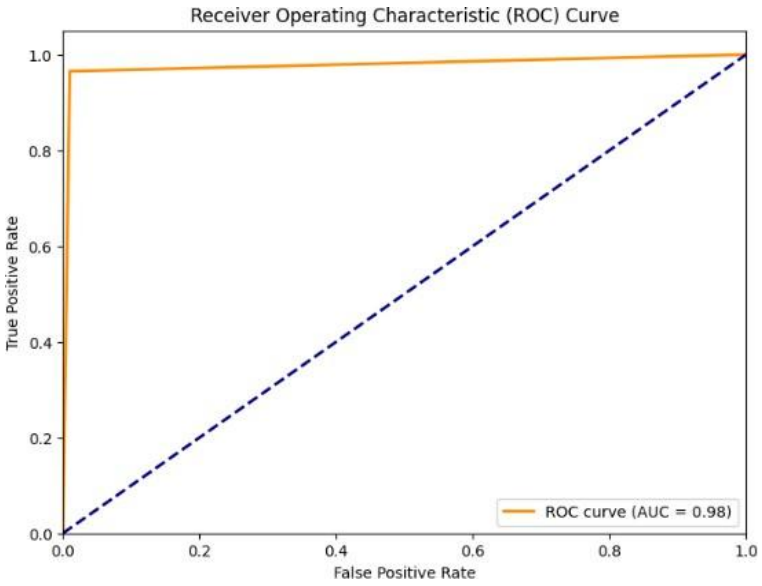

Fig. 10. Roc Curve (RSXG - Random Forest Regressor, XG Boost Regressor, Support Vector Regressor)

Figure 10 showcases the ROC curve for Model 4, achieving an AUC of 0.98. The model exhibits strong predictive capabilities, closely resembling Model 2 in performance, with minimal false positive rates and high classification accuracy.

E. Deployment Phase

The deployment phase of this research focuses on transitioning the developed water quality prediction model from an experimental setting to a functional application. This involves integrating the optimized ensemble model into a user-friendly interface, enabling real-time predictions based on input water quality parameters. The deployment ensures that the proposed solution is not only theoretically robust but also practically implementable for real-world water quality assessment and management.

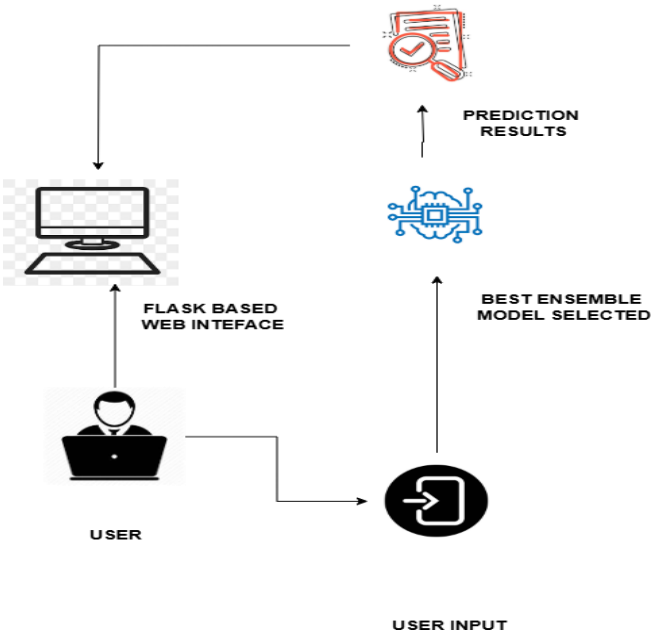

Fig. 11. Deployment Architecture

Figure 11 illustrates the deployment phase of the proposed Water Quality Index (WQI) Prediction System. The best-performing ensemble model, identified through rigorous evaluation, is saved and integrated into a Flask server for real-time prediction. The Flask framework serves as a lightweight deployment solution, allowing users to input water quality parameters through a web-based interface. Upon receiving input, the trained model processes the data and provides the predicted WQI value. This approach ensures accessibility, ease of use, and efficient interaction between the model and end users.

Fig. 12. Water Quality Index Prediction Interface (Flask Based Web Interface)

Fig. 13. WQI Analysis and Awareness Page

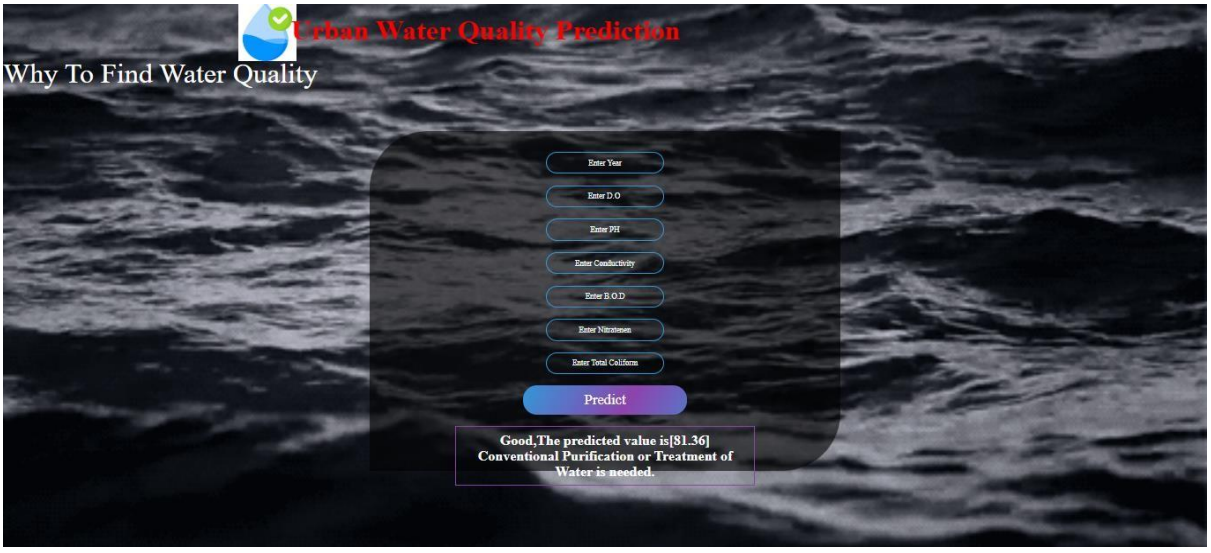

Fig. 14. Prediction Results Page

Figure 12 illustrates the main web-based user interface of the proposed water quality prediction system. This interface enables users to input relevant water quality parameters such as Dissolved Oxygen (D.O.), pH, Conductivity, Biological Oxygen Demand (B.O.D.), Nitrate, and Total Coliform. Upon entering the values, the system loads the pre-trained ensemble model and predicts the Water Quality Index (WQI) value.

Figure 13 presents the WQI index value analysis and awareness section, which provides an interpretative guide for users based on the predicted WQI value. This section categorizes water quality into different ranges, indicating whether water is fit for drinking, cooking, or irrigation purposes, and whether purification or treatment is necessary.

Figure 14 displays the output prediction result generated after the user provides input and presses the "Predict" button. The model processes the input data and outputs the predicted WQI value, along with a textual interpretation of the result, guiding users on the necessary steps regarding water usability. The deployed system effectively integrates an optimized feature selection process, an ensemble learning-based predictive model, and an interactive interface to provide accurate and actionable insights into water quality assessment.

The deployed system is designed to deliver fast and accurate predictions, making it suitable for real-world water quality monitoring applications. By utilizing Flask, the model is hosted in a minimalistic yet effective environment, ensuring scalability and adaptability. The web interface facilitates seamless interaction, enabling users to analyse water quality data effortlessly. This deployment strategy enhances the practical applicability of the proposed system, providing a user-friendly and efficient decision-support tool for environmental management.

V. RESULTS AND DISCUSSION

This section presents the experimental results and a comprehensive analysis of the proposed ensemble models for Water Quality Index (WQI) prediction. The performance of each model is evaluated using key regression metrics, and a comparative analysis is conducted to identify the most effective ensemble approach. Additionally, feature importance analysis using SHAP is discussed to interpret the influence of individual water quality parameters on WQI prediction. The findings highlight the effectiveness of the proposed methodology, demonstrating its potential for real-world water quality assessment and management.

TABLE II. COMPARATIVE ANALYSIS OF EVALUATION METRICS

MODELS	EVALUATION METRICS		
	MSE (Mean Square Error)	MAE (Mean Absolute Error)	R2 SCORE
BASE MODELS EVALUATION			
1. Random Forest Regressor	5.2951	0.8859	0.9711
2. Support Vector Regressor	69.2203	6.2239	0.6227
3. XG Boost Regressor	2.9481	0.6484	0.9839
ENSEMBLE MODEL EVALUATION			
1.RNGB (Random Forest Regressor, Gradient Boosting Regressor, Neural Network)	38.6938	3.9048	0.78907
2.RSGB (Random Forest Regressor, Gradient Boosting Regressor, Support Vector Regressor)	1.4832	0.5685	0.9919

3.RXGB (Random Forest Regressor, Gradient Boosting Regressor, XG Boost Regressor)	3.1126	0.6646	0.9830
4.RSXG (Random Forest Regressor, XG Boost Regressor, Support Vector Regressor)	2.9550	0.6486	0.9839

Table 2 presents the evaluation metrics of both existing models and ensemble models for Water Quality Index (WQI) prediction. Each row represents a different regression model, with its corresponding Mean Squared Error (MSE), Mean Absolute Error (MAE), and R^2 Score, which are used to assess model accuracy and predictive performance. The results indicate that among individual models, XG Boost Regressor achieves the lowest MSE (2.9481) and MAE (0.6484) while attaining the highest R^2 score (0.9839), demonstrating its superior predictive capability over Random Forest and Support Vector Regression (SVR).

In the ensemble model evaluation, the RSGB (Random Forest Regressor, Gradient Boosting Regressor, Support Vector Regressor) combination achieves the best performance with the lowest MSE (1.4832), MAE (0.5685), and the highest R^2 score (0.9919), surpassing all other models. The RSXG ensemble (Random Forest, XG Boost, Support Vector Regressor) follows closely with an R^2 score of 0.9839, similar to XG Boost alone, but does not outperform RSGB. On the other hand, RNGB (Random Forest, Neural Network, Gradient Boosting) performs the worst among ensemble models, with a significantly higher MSE (38.6938) and lower R^2 score (0.78907), indicating a weaker fit to the data. These findings highlight that RSGB is the most optimal ensemble model for WQI prediction, leveraging the strengths of Random Forest, Gradient Boosting, and Support Vector Regression for improved accuracy and robustness.

The comparative analysis reveals that ensemble models generally outperform individual regressors, reinforcing the effectiveness of combining multiple learning techniques. The results also suggest that proper feature selection and ensemble model optimization play a critical role in achieving superior predictive performance for water quality assessment.

```python
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns

# Define model names and evaluation metrics
evaluation_metrics = {
    "RNGB": {"MSE": 38.69388, "MAE": 1.36484, "R2": 0.7890, "AUC": 0.88},
    "RSGB": {"MSE": 1.4832, "MAE": 0.5685, "R2": 0.9919, "AUC": 0.98},
    "RXGB": {"MSE": 3.1126, "MAE": 0.66466, "R2": 0.983, "AUC": 0.98},
    "RSXG": {"MSE": 2.9550, "MAE": 0.64868, "R2": 0.9839, "AUC": 0.98},
}

# Convert dictionary to lists for plotting
model_names = list(evaluation_metrics.keys())
mse_values = [evaluation_metrics[m]["MSE"] for m in model_names]
r2_values = [evaluation_metrics[m]["R2"] for m in model_names]
mae_values = [evaluation_metrics[m]["MAE"] for m in model_names]
auc_values = [evaluation_metrics[m]["AUC"] for m in model_names]

# Function to annotate bars
def annotate_bars(ax, values):
    for i, v in enumerate(values):
        ax.text(i, v + 0.005, f"{v:.3f}", ha='center', fontsize=10)

# Plot MSE
plt.figure(figsize=(8, 5))
ax = sns.barplot(x=model_names, y=mse_values, hue=model_names, palette="Blues", legend=False)
annotate_bars(ax, mse_values)
plt.title("Mean Squared Error (MSE)")
plt.ylabel("MSE")
plt.xticks(rotation=45)
plt.show()

# Plot R² Score
plt.figure(figsize=(8, 5))
ax = sns.barplot(x=model_names, y=r2_values, hue=model_names, palette="Greens", legend=False)
annotate_bars(ax, r2_values)
plt.title("R² Score")
plt.ylabel("R²")
plt.xticks(rotation=45)
plt.show()
```

```python
# Plot MAE
plt.figure(figsize=(8, 5))
ax = sns.barplot(x=model_names, y=mae_values, hue=model_names, palette="Reds", legend=False)
annotate_bars(ax, mae_values)
plt.title("Mean Absolute Error (MAE)")
plt.ylabel("MAE")
plt.xticks(rotation=45)
plt.show()

# Plot AUC
plt.figure(figsize=(8, 5))
ax = sns.barplot(x=model_names, y=auc_values, hue=model_names, palette="Purples", legend=False)
annotate_bars(ax, auc_values)
plt.title("Area Under Curve (AUC)")
plt.ylabel("AUC")
plt.xticks(rotation=45)
plt.show()
```

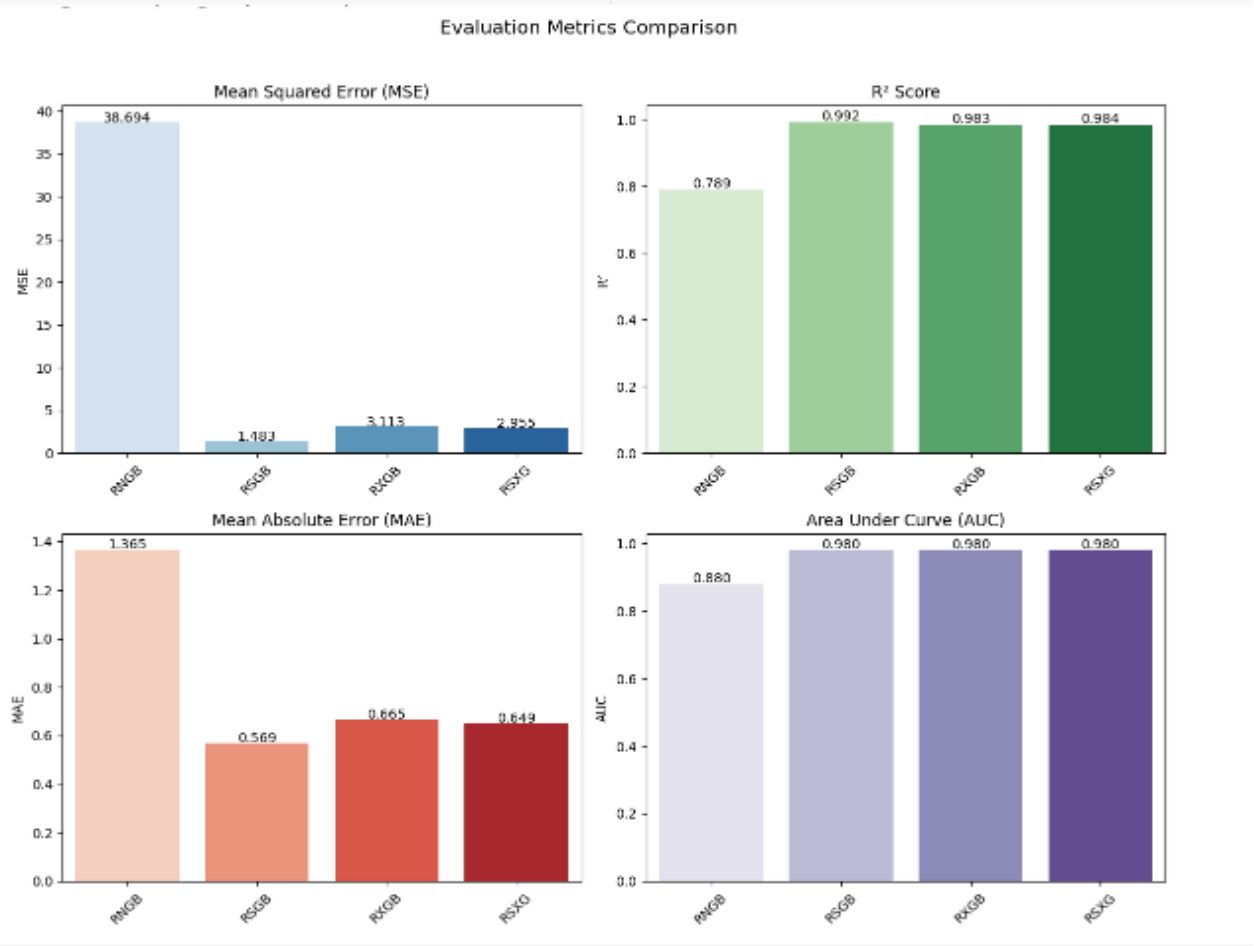

Fig. 15. Comparison of Various Metrics for All Ensemble Models

```python
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns

# Define model names and evaluation metrics
evaluation_metrics = {
    "RNGB": {"MSE": 38.69388, "MAE": 1.36484, "R2": 0.7890, "AUC": 0.88},
    "RSGB": {"MSE": 1.4832, "MAE": 0.5685, "R2": 0.9919, "AUC": 0.98},
    "RXGB": {"MSE": 3.1126, "MAE": 0.66466, "R2": 0.983, "AUC": 0.98},
    "RSXG": {"MSE": 2.9550, "MAE": 0.64868, "R2": 0.9839, "AUC": 0.98},
}

# Convert dictionary to a DataFrame for plotting
import pandas as pd
data = []
for model, metrics in evaluation_metrics.items():
    for metric, value in metrics.items():
        data.append([model, metric, value])

df = pd.DataFrame(data, columns=["Model", "Metric", "Value"])

# Create a single bar plot
plt.figure(figsize=(12, 6))
sns.barplot(x="Model", y="Value", hue="Metric", data=df)

# Annotate bars
for p in plt.gca().patches:
    plt.gca().annotate(f"{p.get_height():.3f}", (p.get_x() + p.get_width() / 2., p.get_height()),
                       ha='center', va='bottom', fontsize=10, color='black')

plt.title("Comparison of Evaluation Metrics Across Models")
plt.ylabel("Metric Value")
plt.xticks(rotation=45)
plt.legend(title="Metrics")
plt.show()
```

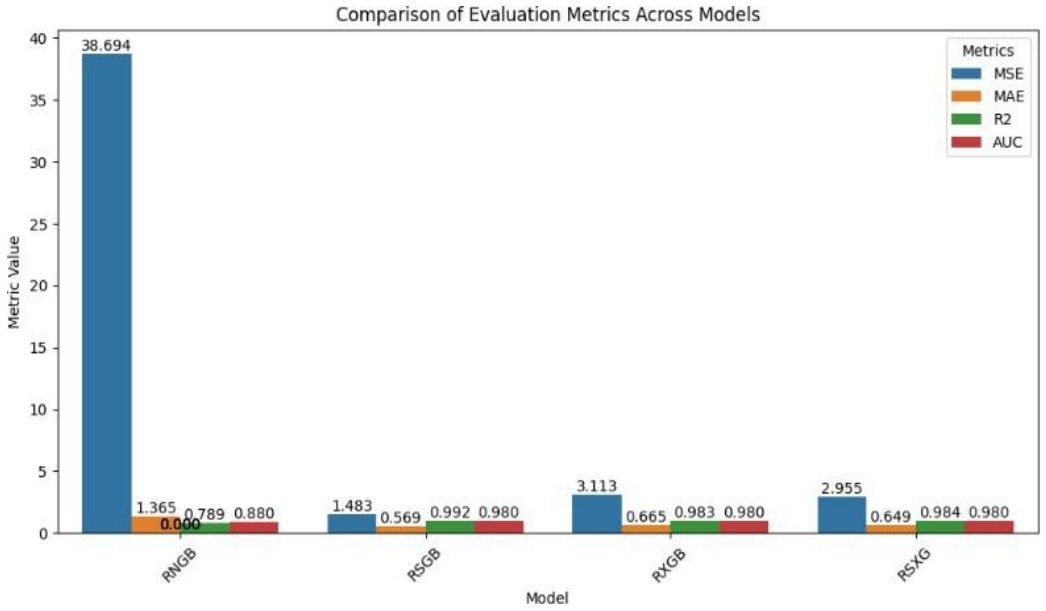

Fig. 16. Overall Comparison of Metrics and Ensemble Models

Figure 15 presents a comparative analysis of evaluation metrics, including Mean Squared Error (MSE), Mean Absolute Error (MAE), R^2 Score, and Area Under the Curve (AUC) for different ensemble models. The RSGB model, which combines Random Forest Regressor, Gradient Boosting Regressor, and Support Vector Regressor, outperforms other models with the lowest MSE (1.4832) and MAE (0.5685), as well as the highest R^2 Score (0.9919), indicating superior predictive accuracy. In contrast, the RNGB model exhibits the highest error metrics, suggesting that the inclusion of Neural Networks may not be optimal for this dataset.

Figure 16 provides an overall comparison of the evaluation metrics across all ensemble models. The RSGB model consistently demonstrates the best performance, closely followed by RXGB and RSXG. The RSXG model also shows competitive results with a high R^2 Score (0.9839) and low MAE (0.6486). These results reinforce the effectiveness of ensemble learning in improving water quality prediction, with RSGB emerging as the most robust model for this regression task.

The proposed ensemble models significantly improve water quality prediction compared to existing individual models. The RSGB model achieves the lowest MSE and MAE while attaining the highest R^2 Score, demonstrating its robustness in handling non-linear relationships and complex dependencies within the dataset. Compared to traditional models like Support Vector Regressor and Random Forest Regressor, the ensemble approach enhances predictive accuracy and reduces error rates. However, while the model performs well, potential limitations include dataset constraints and the exclusion of additional environmental factors that could further refine predictions. Future research can incorporate advanced deep learning techniques or hybrid models, integrating real-time data sources to enhance model generalization and adaptability for broader applications in water quality monitoring.

TABLE III. COMPARATIVE ANALYSIS OF EXISTING WORKS

STUDY	DATASET PARAMETERS USED	FINDINGS
Advanced ML Models for Robust Prediction of Water Quality [13]	pH, Temperature, DO, BOD, Nitrate, Fecal Coliform, Total Coliform, Turbidity	This study utilizes advanced ML models like Random Forest, XG Boost, and Neural Networks for predicting water quality. Feature selection methods were applied to improve model accuracy. The Random Forest model achieved the best results with an R^2 score of 0.95.
Water Quality Prediction Using Machine Learning [14]	pH, DO, BOD, Nitrate, Total Coliform, Turbidity, Conductivity	This study compared multiple static models (SVM, Decision Trees, Gradient Boosting) for water quality analysis. The Gradient Boosting model performed best, with an MSE of 3.25 and R^2 of 0.92. The study highlights the role of feature importance in prediction accuracy.
Water Quality Prediction – A Data-Driven Approach [15]	pH, DO, BOD, Nitrate, Total Coliform, TDS, Conductivity	This research implements an ensemble approach combining Random Forest, Gradient Boosting, and Neural Networks to improve predictive performance. The ensemble model achieved an R^2 score of 0.96, outperforming individual models. The study suggests that adding conductivity and TDS parameters mproves predictions.

Table III presents a comparative analysis of existing studies on water quality prediction models, focusing on dataset parameters, model types, evaluation metrics, and predictive performance. The dataset parameters commonly used across studies include pH, Dissolved Oxygen (DO), Biological Oxygen Demand (BOD), Nitrate, and Total Coliform, which are also fundamental in our research work. However, certain studies incorporated Conductivity and Total Dissolved Solids (TDS) to enhance prediction accuracy, which can be considered for future improvements.

From the evaluation metrics, it is evident that ensemble models consistently outperform individual models, as demonstrated, where an ensemble of Random Forest, Gradient Boosting, and Neural Networks achieved the highest R^2 score of 0.96. Similarly, our research work integrates Recursive Feature Elimination (RFE) and SHAP- based feature selection techniques, further refining model performance. Our best ensemble model (RSGB) achieved an R^2 score of 0.9919, surpassing the reported models in related works. This highlights the effectiveness of combining optimized feature selection with ensemble modeling to achieve superior predictive accuracy.

VI. CONCLUSION AND FUTURE WORK

Based on this work's comparative analysis and findings, we conclude that the ensemble-based regression model incorporating Recursive Feature Elimination (RFE) and SHAP-based analysis is a reliable and effective approach for Water Quality Index (WQI) prediction. Among the tested ensemble models, the combination of Random Forest Regressor, Gradient Boosting, and Support Vector Regression (Model 2) achieved the best performance across multiple evaluation metrics. The integration of explainability techniques such as SHAP allows for a deeper understanding of the contribution of each feature, aiding policymakers and environmental researchers in informed decision-making.

The findings from our study demonstrate that incorporating advanced feature selection techniques (RFE and SHAP) and ensemble learning significantly improves water quality prediction accuracy. Comparative analysis with existing models confirms that our proposed ensemble approach yields superior performance in terms of MSE, MAE, and R^2 score. The results validate the potential of integrating multiple machine learning models for robust and interpretable water quality assessment.

Future work can explore deep learning models or hybrid ensemble frameworks to improve predictive performance and generalization. Additionally, real-time data acquisition through IoT-enabled sensors and integrating external environmental factors such as climate and land use patterns could enhance the model's applicability and robustness for large-scale water quality assessment.

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