

# **Prediction of Water Quality Index Using Machine Learning Algorithms**

**by**

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## 1 Introduction

Water is essential for human well-being and socio-economic development [1]. According to the 2021 World Water Development Report by UNESCO, global freshwater usage has increased sixfold in the last century and continues to grow by 1% annually [2]. This increase is driven by factors like population growth, economic development, and evolving consumption habits [2]. However, this increased water consumption poses significant challenges in maintaining water quality. Activities such as industrialization, agriculture, and urbanization have led to environmental degradation and water pollution, with profound implications for human health and sustainable development [3]. Thus, it's imperative to monitor and assess water quality rigorously to protect both human health and the environment, facilitating effective and sustainable water management.

Water Quality Index (WQI) is a mathematical model by converting large quantities of water quality data into a single value, making it easier to understand and monitor the overall quality of water resources [4, 5]. The WQI comprises four processes that include parameter selection, sub-Index calculation, weighting factor determination, and sub-Indices aggregation. First process involves choosing which water quality parameters to include in the evaluation. Once the parameters are selected, actual water quality data is collected. For each chosen parameter, the concentrations found in the water samples are converted into a single numerical value. These values help create sub-indices, which are essentially scores or ratings for each parameter. Third, weighting factor is assigned to each parameter to reflect their significance. Parameters with more impact on water quality receive higher weights in the calculation. Finally, an aggregation function combines all the sub-indices by using the assigned weighting factors for each parameter. This process generates a final single numerical value - the WQI. [6-9].

WQI might not provide an entirely accurate assessment of water quality. The reason being that each index is typically designed for certain locations or types of water, making it biased towards those specific conditions. Additionally, these indices can be highly sensitive to specific parameters concentrations or heavily reliant on the assigned weights for these parameters, which can affect the overall assessment of water quality [4, 6]. To address these problems, there's a critical need for an alternative approach that ensures both computational efficiency and accuracy in estimating the WQI [10]. In recent years, machine learning (ML) techniques provides an alternate method to estimate the WQI based on existing data [4, 11].

The primary goal of this study is to develop an efficient method for predicting the WQI, a single metric that encompasses both the Water Quality Classification (WQC) and the overall

quality of water. Our aim is to streamline the process of water quality assessment, thereby saving time and resources typically required for manual measurements. We achieved this by utilizing regression learning techniques such as Linear Regression, Random Forest Regression, XGBoosting regression. These techniques applied to predict WQI based on key parameters including dissolved oxygen, nitrite, nitrate, total nitrogen, total phosphorus, total suspended solids, biological oxygen demand, and turbidity.

## 2 Data Wrangling

The original water quality dataset was loaded from a CSV file into a Pandas DataFrame named `q_data`. It contains 18148 rows and 48 columns with varying data types, missing values, and unclear column names. To prepare for WQI calculation, relevant columns were selected and renamed for clarity. Numeric conversions were applied to certain columns, such as 'TP (mg/L)', to facilitate analysis. Additionally, adjustments were made to the 'Date' column, converting it to datetime format for temporal analysis.

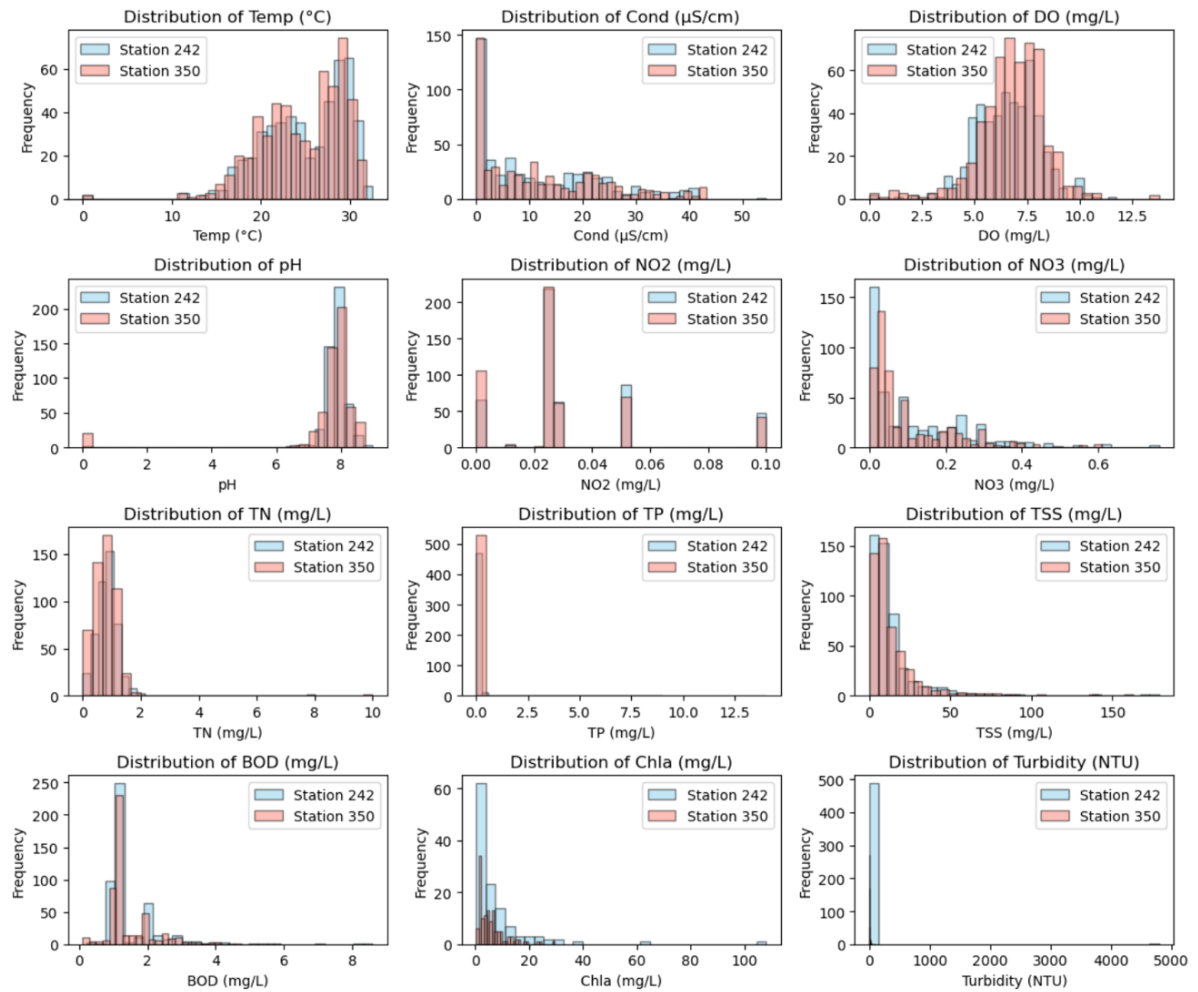
The modeling process specifically targeted river water quality, so the analysis was streamlined to exclusively include records pertaining to river water samples, which consist of 1068 rows and 15 columns. Addressing missing data, calculations were performed to determine the number and percentage of missing values for each column. Columns with a high percentage of missing values, such as 'Chla (mg/L)' (76.50%), were removed from the dataset to enhance data reliability. Furthermore, zero values in the 'Temp (°C)' and 'pH' columns were replaced with NaN to rectify potential inaccuracies. Erroneous TN, TP, and Turbidity values were identified and corrected, bolstering the dataset's accuracy. Imputing NaN values with the median for selected columns further optimized data quality.

The WQI was computed using weighted arithmetic methods, incorporating standard desirable and ideal values for various parameters. This facilitated the quantification of water quality for each station, providing valuable insights into overall water health. Classification functions were applied to categorize WQI into distinct water quality classes, aiding in interpretation and decision-making.

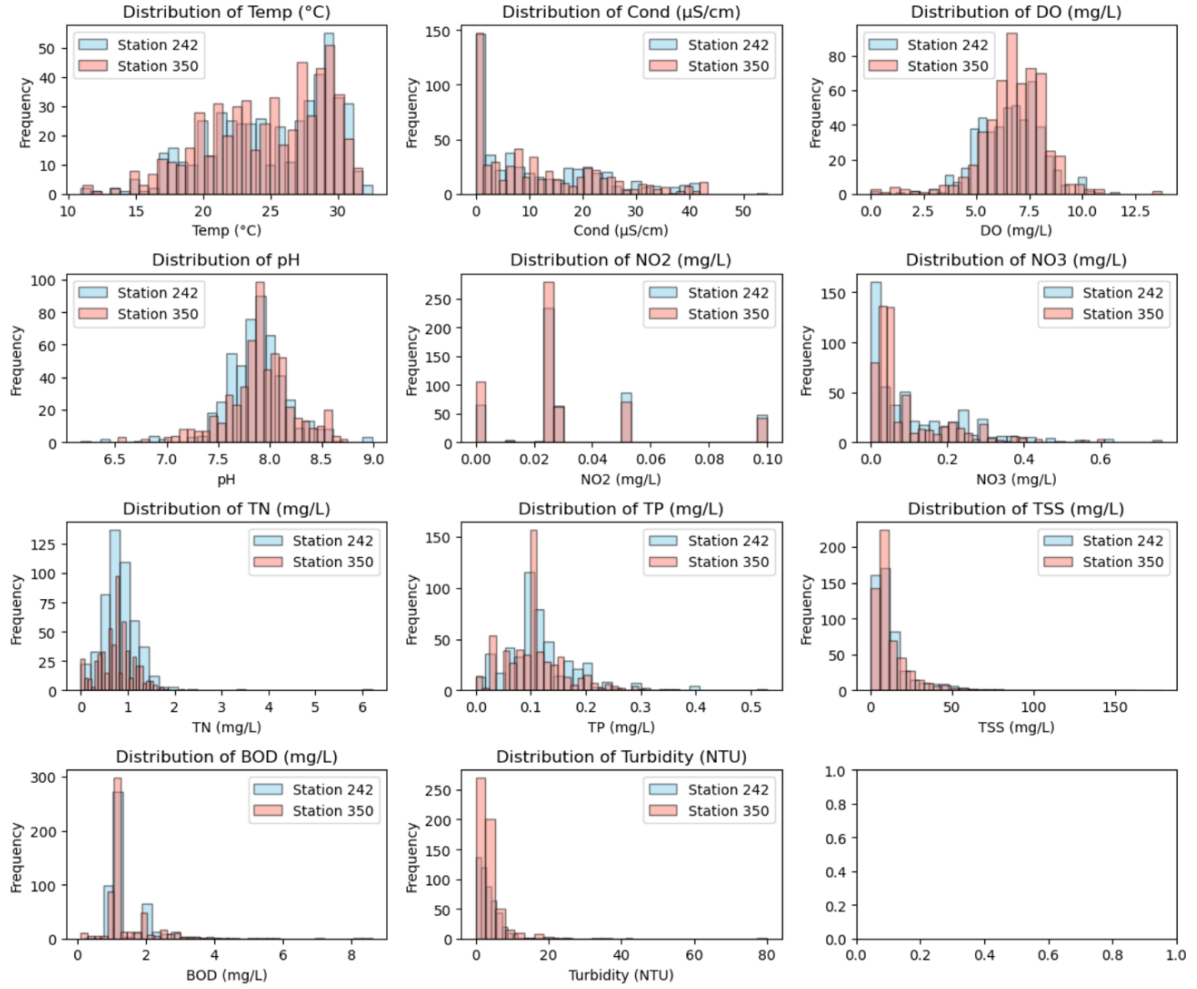
Lastly, the processed data, focusing on river water samples, was stored in a CSV file, named "water\_quality\_index.csv," ensuring accessibility for future analyses.

Distribution of data before and after processing is provided in Figure 1 and 2. Figure 1 illustrates the distribution of data before processing, where no adjustments were made to missing values or outliers. Figure 2 displays the distribution of data after preprocessing,

where missing values were handled, outliers were addressed, and necessary transformations were applied.



**Figure 1.** Distribution of data before processing.



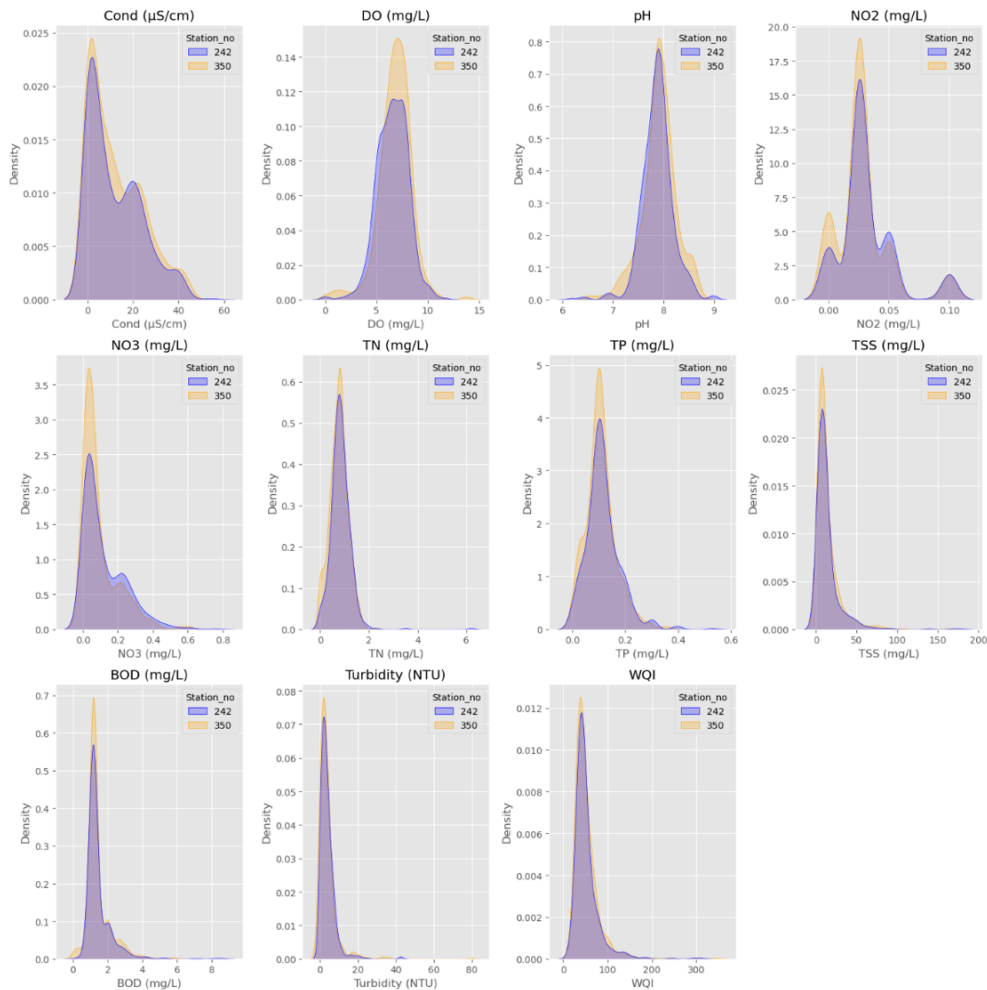
**Figure 2.** Distribution of data after processing.

### 3 Exploratory Data Analysis (EDA)

In the EDA phase, duplicate records were first identified and removed based on a subset of columns relevant to water quality parameters, such as conductivity, dissolved oxygen, pH, nitrite, nitrate, total nitrogen, total phosphorus, total suspended solids, biological oxygen demand, and turbidity. Following the removal of duplicate values, the DataFrame `wqi` comprises of 1025 rows and 14 columns. Additionally, outliers were observed in certain numerical features, indicating potential errors in data collection or measurement.

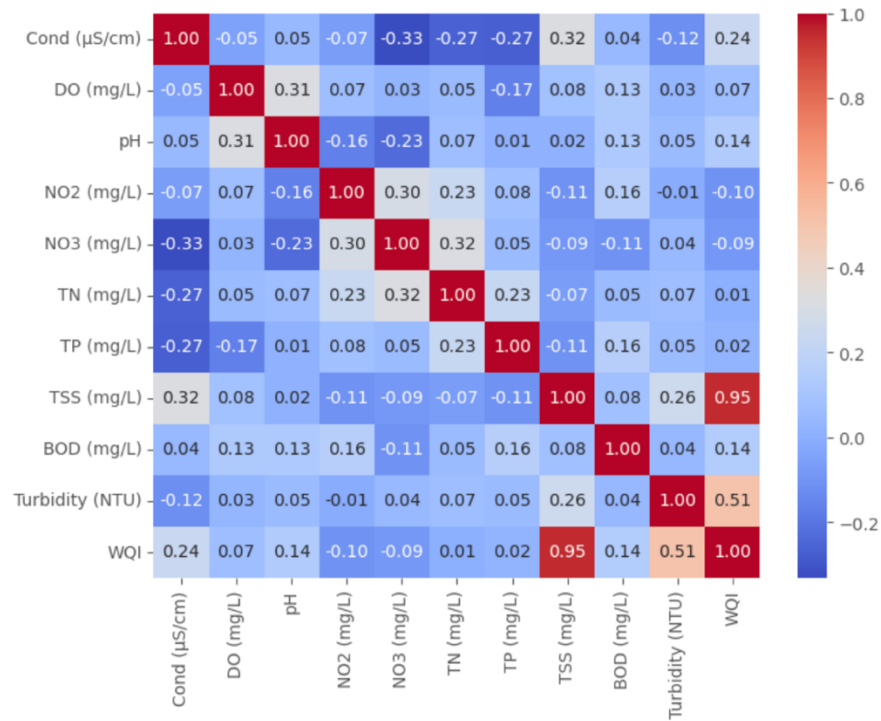
Subsequently, the distribution of numerical features was explored through histograms and kernel density estimation (KDE) plots (Figure 3). Skewed distributions were observed in several features, suggesting a concentration of values on one side of the distribution. Moreover, multimodal distributions were identified in certain features (NO<sub>2</sub>), indicating the

presence of distinct groups or clusters within the data. By examining the KDE of the WQI, it was evident that the distribution of WQI values was right-skewed, with most data concentrated between 35 and 56. The KDE also revealed that the range of WQI values spanned from 12.5 to 343, indicating a wide variability in water quality across the dataset. Additionally, the mean WQI value was approximately 51, suggesting a moderate overall water quality level.



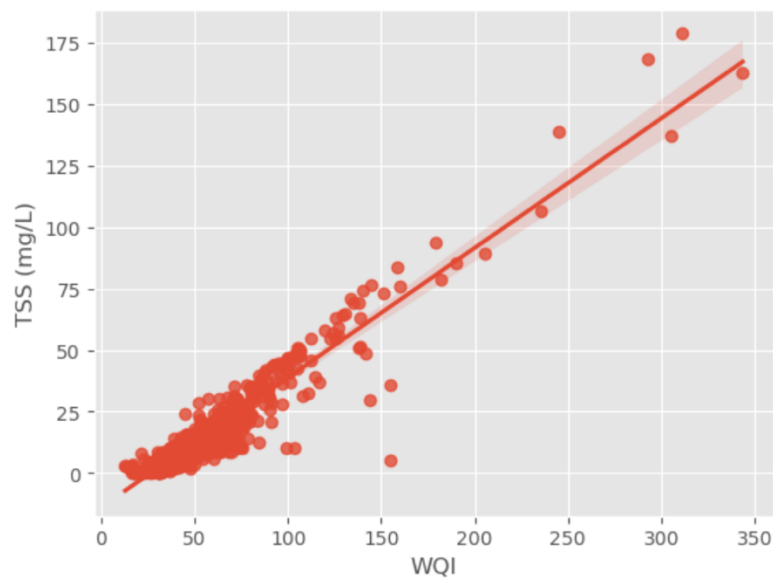
**Figure 3.** KDE plots for numerical features for each station.

To understand the relationships between numerical features and the WQI, pairplots, scatterplots, and regression plots were generated. Additionally, the correlation heatmap provides an overview of the relationships between different numerical features in the dataset (Figure 4). WQI has a very strong positive correlation with TSS and a moderate positive correlation with Turbidity, indicating that higher values of these parameters are associated with poorer water. The correlations with other variables are weak (Cond, pH, NO<sub>2</sub>, NO<sub>3</sub>, BOD) or very weak (DO, TN, TP).



**Figure 4.** Correlation heatmap of numerical features.

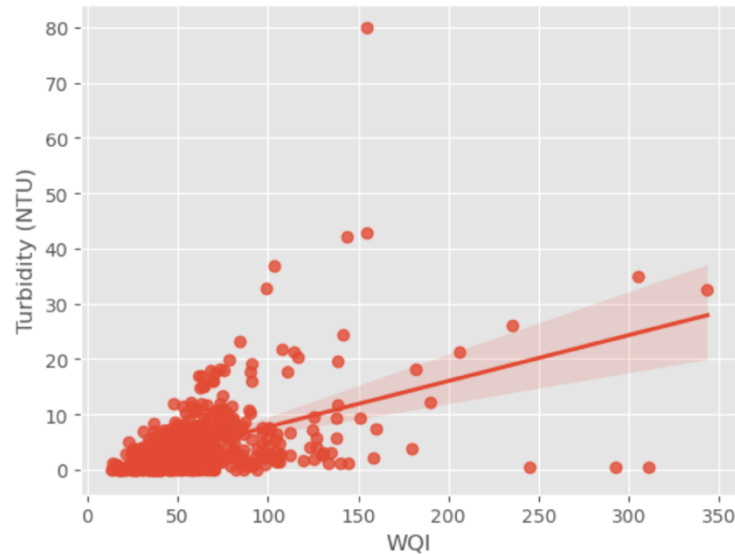
In Figure 5, it is evident that as TSS increase, the WQI tends to increase as well, and vice versa. Despite the presence of outliers in the data, the positive correlation line in the scatter plot suggests that these outliers may not fundamentally alter the relationship between the variables. Knowing the value of TSS can provide valuable information for predicting WQI levels in water samples.



**Figure 5.** Relationship between the 'WQI' and 'TSS (mg/L)'.



Figure 6 illustrates the relationship between the 'WQI' and 'Turbidity (NTU)'. Even though the relationship between turbidity and WQI may not be perfectly linear, the general trend indicates that as turbidity increases, the corresponding WQI tends to increase as well. This suggests that higher levels of turbidity are associated with poorer water quality, as indicated by higher WQI values. While the correlation between WQI and turbidity may not be very strong, turbidity can still provide valuable information for predicting WQI levels in water samples.



**Figure 6.** Relationship between the 'WQI' and 'Turbidity (NTU)'.

#### 4 Preprocessing and Training Data Development

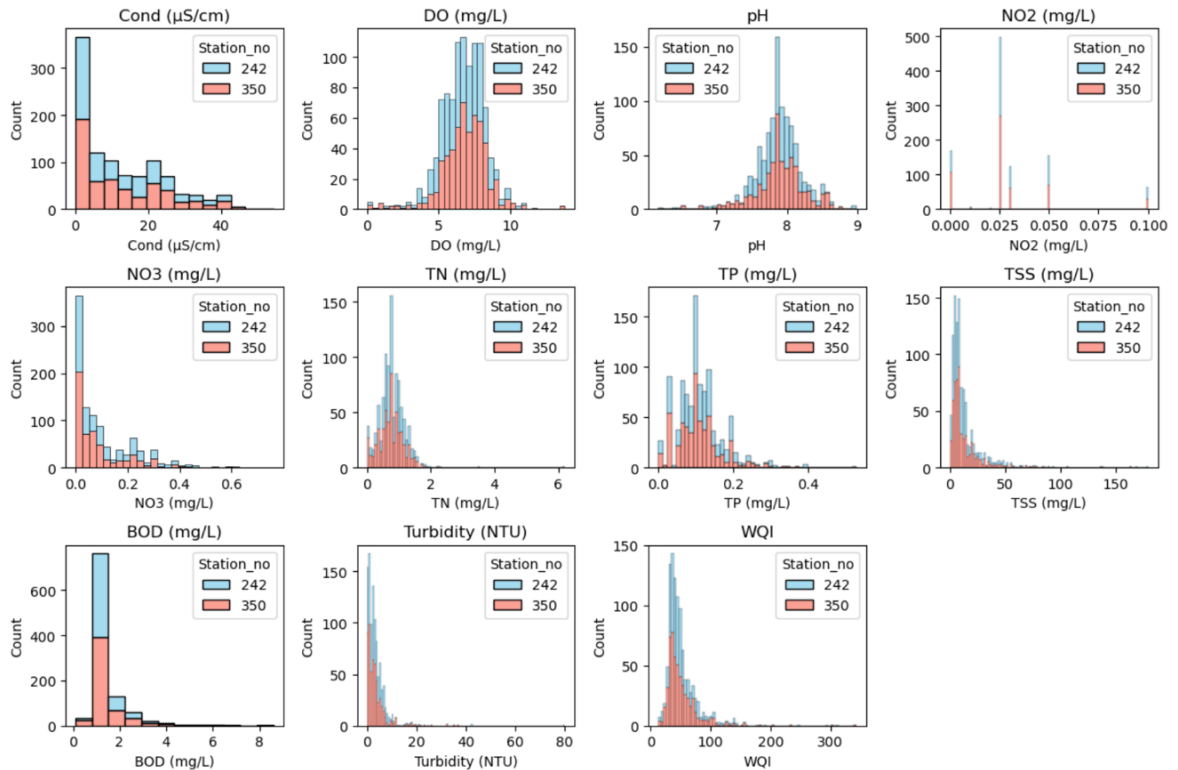
In the preprocessing phase, the water quality dataset was initially loaded from a CSV file, and its dimensions were examined to confirm the number of rows and columns. Additionally, the data types were checked, and it was verified that there were no missing values. Subsequently, several transformation steps were applied to prepare the data for analysis. The 'Date' column was converted to datetime format to facilitate time-based analysis, while the categorical variable 'Water Quality Classification' was encoded into binary columns using one-hot encoding. Furthermore, the 'Month' column was extracted from the 'Date' column to investigate potential seasonal patterns in the data.

Following data splitting into training and testing sets with an 80-20 ratio, the features ('X') and target variable ('y') were defined. The next steps focused on feature scaling and transformation to ensure consistency and reduce skewness or outliers in the numerical

features. Power Transformation was applied to address skewness and outliers, while MinMaxScaler was used to scale all numerical features to a range between 0 and 1.

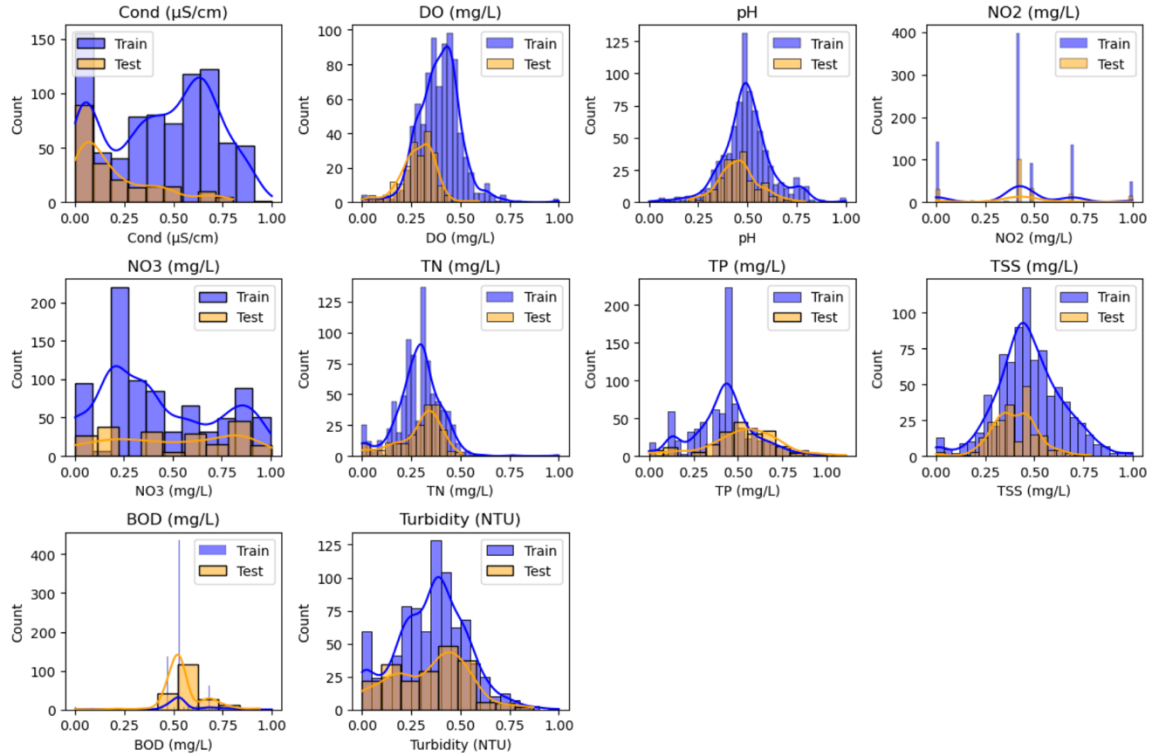
Finally, the transformed training and testing data were saved to CSV files ('X\_train\_transformed.csv' and 'X\_test\_transformed.csv'), along with the unchanged target variables ('y\_train.csv' and 'y\_test.csv').

To visually assess the effects of preprocessing, histograms of numerical features were plotted before and after scaling (Figure 7 & 8). Before scaling, features such as Cond, NO3, TSS, BOD, and Turbidity exhibit skewed distributions (Figure 7). Conversely, DO, pH, TN, and TP demonstrate distributions closer to normal. NO2 appears to have irregular sampling intervals, resulting in gaps between data points. For instance, some data are recorded at intervals of 0, 0.025, 0.050, and 0.1. The scale of each feature varies, with DO measure in mg/L and Cond in  $\mu\text{S/cm}$ , contributing to differences in their value ranges. Some features have a narrow range, with closely clustered values, while others exhibit a wider spread, indicating greater variability. Additionally, the central tendency of the features varies, with some showing higher average values than others.



**Figure 7.** Histograms of numerical features before scaling.

After applying MinMaxScaler to the numerical features in the dataset, we observed that all parameters now exhibit distributions closer to a normal distribution (Figure 8). Additionally, the scaling process has successfully transformed the features to a consistent range between 0 and 1. Additionally, the 'Station\_no' and 'Month' columns were concatenated with the transformed dataframes to preserve contextual information for further analysis.



**Figure 8.** Histograms of numerical features after scaling.

## 5 Modeling

Several regression models were selected for predicting the WQI based on the given features. These models included Linear Regression, Lasso Regression, Ridge Regression, Random Forest Regression, and XGBoost Regression. Each model was trained using the training data and evaluated using the testing data to assess its performance. Evaluation metrics such as R-squared (R<sup>2</sup>) score, Mean Squared Error (MSE), and Mean Absolute Error (MAE) were used to quantify the performance of each model.

To optimize the performance of Random Forest Regression and XGBoost Regression, hyperparameter tuning was performed using GridSearchCV. This involved systematically searching through a range of hyperparameters to find the combination that yielded the best

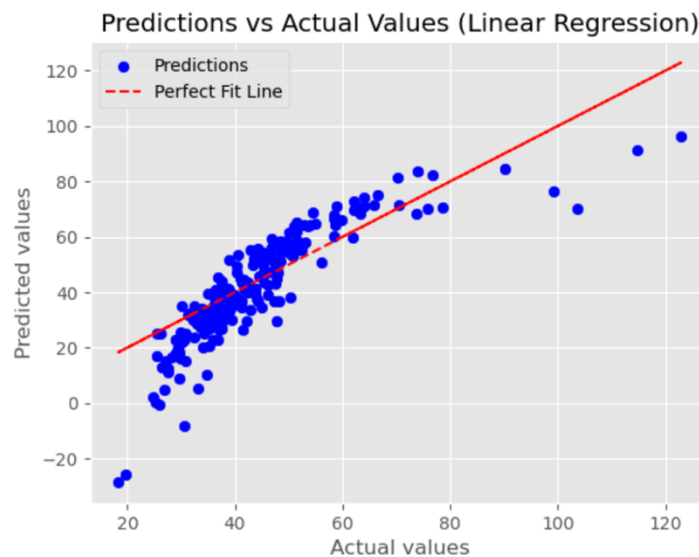
performance for each model. Hyperparameters tuned included the 'n\_estimators': [100, 200, 300], 'max\_depth': [None, 10, 20], 'min\_samples\_split': [2, 5, 10], 'min\_samples\_leaf': [1, 2, 4], and 'max\_features': ['sqrt', 'log2'] for Random Forest, 'n\_estimators': [100, 200, 300], 'max\_depth': [3, 5, 7], 'learning\_rate': [0.01, 0.05, 0.1] for XGBoost.

Cross-validation was employed to assess the models' performance across different splits of the data. This technique helps estimate how the models will perform on unseen data and provides insights into their stability and generalization ability. Various folds (e.g., 3-fold, 5-fold, 7-fold, 10-fold) were used to evaluate the models' performance under different scenarios.

Scatter plots were used to compare predicted vs. actual values, while line plots were used to display best scores and cross-validation scores across different folds. These visualizations aided in understanding the models' performance and conveying insights effectively.

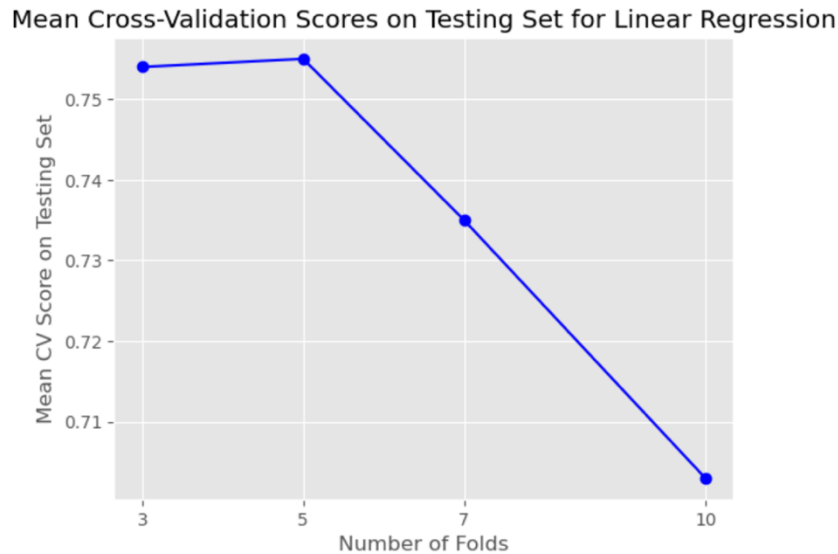
## 5.1 Linear Regression

The **Linear Regression** model achieved an **R2** value of approximately **0.477** on the testing set. This indicates that around 47.75% of the variance in the target variable (WQI) is explained by the features in the model. The **MSE** on the testing set is approximately **117.107**, which provides a measure of the average squared difference between the actual and predicted WQI values. The **MAE** on the testing set is approximately **8.069**, representing the average absolute difference between the actual and predicted WQI values.



**Figure 9.** Relationship between the predicted and actual values generated by the Linear Regression model.

The scatter plot illustrates the relationship between the predicted and actual values generated by the Linear Regression model (Figure 9). Each point on the plot represents a pair of actual and predicted values for the WQI. The red dashed line represents a perfect fit, where the predicted values would perfectly align with the actual values. However, the scatter of points deviates from this ideal line, indicating that the model's predictions do not precisely match the actual values. This suggests that the Linear Regression model may not fully capture the underlying complexities of the data, leading to some degree of prediction error.



**Figure 10.** The cross-validation results for the Linear Regression model.

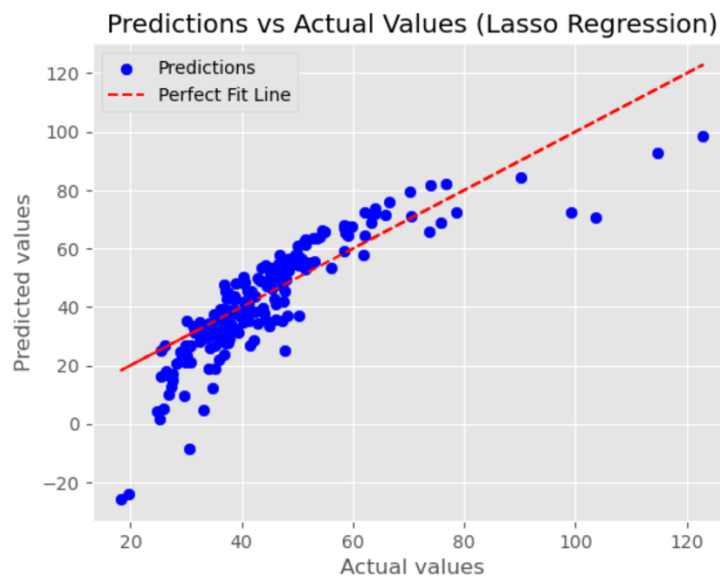
The cross-validation results for the Linear Regression model, indicate varying levels of performance across different numbers of splits, is shown in Figure 10. As the number of folds increases from 3 to 10, the mean cross-validation score on the training set tends to increase gradually, indicating better model performance as more data is used for training. However, the mean cross-validation score on the testing set does not exhibit a consistent trend. It peaks at 5-fold cross-validation and slightly decreases for 7-fold and 10-fold cross-validation. The standard deviation in cross-validation scores on the testing set increases as the number of folds increases, suggesting higher variability in model performance when evaluated on different subsets of the data. Overall, 5-fold cross-validation yields the highest mean cross-validation score (0.755) on the testing set, indicating that it strikes a good balance between model performance and stability. However, the differences in mean scores between different numbers of folds are relatively small, suggesting that the choice of the number of folds may not significantly impact model performance in this case.

## 5.2 Lasso Regression

The **Lasso regression** model achieved an **R<sup>2</sup>** value of approximately **0.536** on the testing set. This indicates that the Lasso model explains about 53.6% of the variance in the target variable, WQI, which is higher than the R<sup>2</sup> value obtained from the Linear Regression model. Additionally, the Lasso model yielded a **MSE** of approximately **103.36** and a **MAE** of approximately **7.438** on the testing set. Both metrics are lower compared to those obtained from the Linear Regression model, suggesting that the Lasso model provides better predictions and has lower prediction errors.

Overall, based on these metrics, the Lasso regression model seems to perform better than the Linear Regression model for this dataset.

The scatter plot visually represents the relationship between the predicted and actual values generated by the Lasso regression model (Figure 11). While there's some dispersion around the ideal diagonal line, indicating variability in predictions, the general trend shows a moderate alignment between predicted and actual WQI values. Despite not achieving perfect accuracy, the Lasso model captures a substantial portion of the variance in WQI values, as indicated by the trend observed in the scatter plot.



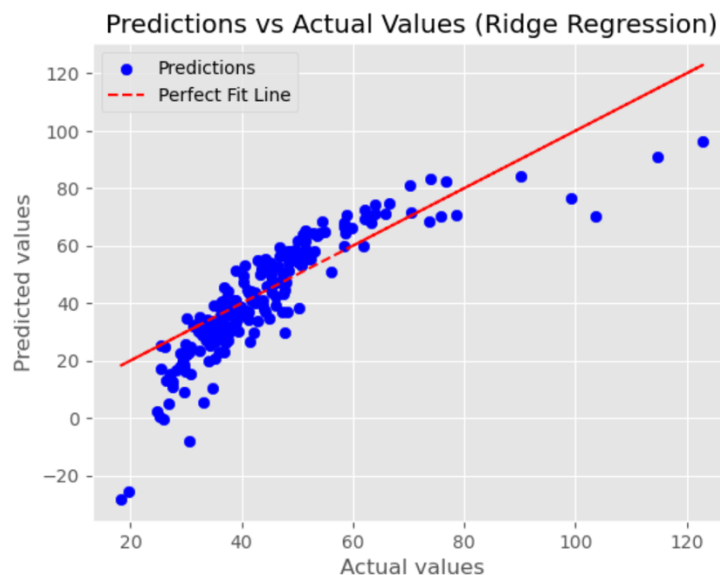
**Figure 11.** Relationship between the predicted and actual values generated by the Lasso Regression model.

### 5.3 Ridge Regression

The **Ridge regression** model achieved an **R2** value of approximately **0.481** on the testing set. This indicates that the Ridge model explains about 48.1% of the variance in the target variable, WQI, which is comparable to the R2 value obtained from the Linear Regression model but slightly lower than the R2 value obtained from the Lasso model. Additionally, the Ridge model yielded a **MSE** of approximately **116.024** and a **MAE** of approximately **8.032** on the testing set. These error metrics are slightly lower than those obtained from the Linear Regression model but slightly higher compared to those obtained from the Lasso model.

Overall, the Ridge regression model performs similarly to the Linear Regression model and slightly worse than the Lasso model in terms of R2 value and prediction errors. Therefore, the Lasso model may still be the preferable choice for this dataset based on these evaluation metrics.

The scatter plot shows how well the Ridge regression model's predictions match the actual values (Figure 12). Ideally, all points would fall exactly on the red dashed line, indicating a perfect match. However, we see some spread, suggesting that the model's predictions don't perfectly align with reality. This indicates that while the Ridge regression captures some patterns, it may miss others.



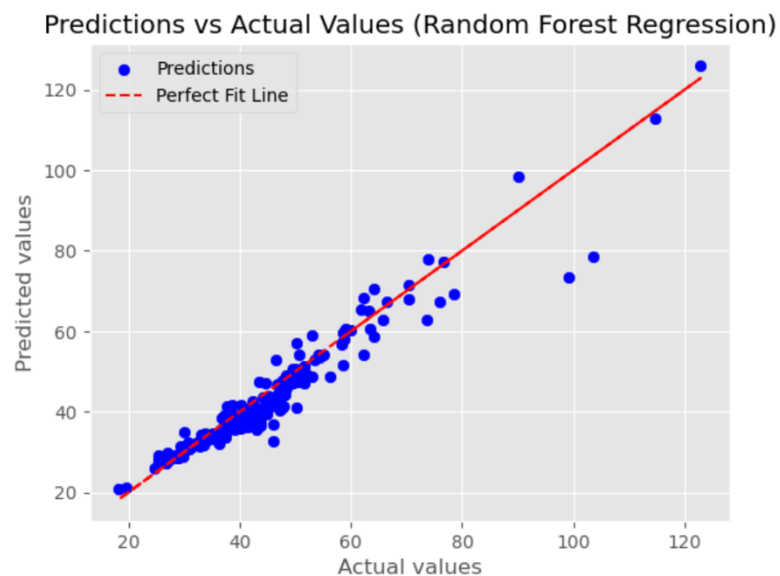
**Figure 12.** Relationship between the predicted and actual values generated by the Ridge Regression model.

## 5.4 Random Forest Regression

The **Random Forest** regression model achieved an impressive **R<sup>2</sup>** value of approximately **0.923** on the testing set. This indicates that the Random Forest model explains about 93.3% of the variance in the target variable, WQI, which is significantly higher than the R<sup>2</sup> values obtained from the Linear Regression, Lasso Regression, and Ridge Regression models. Additionally, the Random Forest model yielded a **MSE** of approximately **17.285** and a **MAE** of approximately **2.665** on the testing set. These error metrics are substantially lower compared to those obtained from the other regression models, indicating that the Random Forest model provides highly accurate predictions for the WQI.

Overall, the Random Forest Regression model demonstrates superior performance in terms of R<sup>2</sup> value and prediction errors, making it the preferred choice for this dataset.

The scatter plot for Random Forest shows that the predicted values closely follow the trend of the actual values, indicating a strong correlation between the predicted and actual values (Figure 13). Additionally, most of the points are clustered near the perfect fit line, suggesting that the model's predictions are accurate and align well with the ground truth.



**Figure 13.** Relationship between the predicted and actual values generated by the Random Forest model.

Table 1 provides an overview of the Random Forest cross-validation results, including the maximum depth, maximum features, number of estimators, the best score achieved, mean cross-



validation scores on testing sets, and the standard deviation in cross-validation scores on the testing set.

**Table 1.** Random Forest Model Cross-Validation Results.

	Cross-Validation	Max Depth	Max Features	N_Estimators	R-squared Score	Mean CV Score (Testing Set)	Standard Deviation
0	3-fold	20.0	log2	NaN	0.857	0.739	0.080
1	5-fold	20.0	sqrt	300.0	0.880	0.774	0.083
2	7-fold	NaN	log2	NaN	0.906	0.770	0.116
3	10-fold	20.0	log2	200.0	0.909	0.781	0.103

In the 3-fold cross-validation scenario, the best estimator was identified with a `max_depth` of 20 and `max_features` set to 'log2', achieving an R-squared score of approximately 0.857. Despite this relatively high score, the mean cross-validation score on the testing set was approximately 0.739, exhibiting a standard deviation of around 0.080, suggesting some variability in model performance.

Expanding the analysis to a 5-fold cross-validation, the best estimator retained the same `max_depth` parameter but changed the `max_features` to 'sqrt', with 300 estimators. This adjustment led to an improvement in the R-squared score to approximately 0.880. Furthermore, the mean cross-validation score on the testing set was raised to approximately 0.774, accompanied by a standard deviation of about 0.083, indicating enhanced stability compared to the 3-fold case.

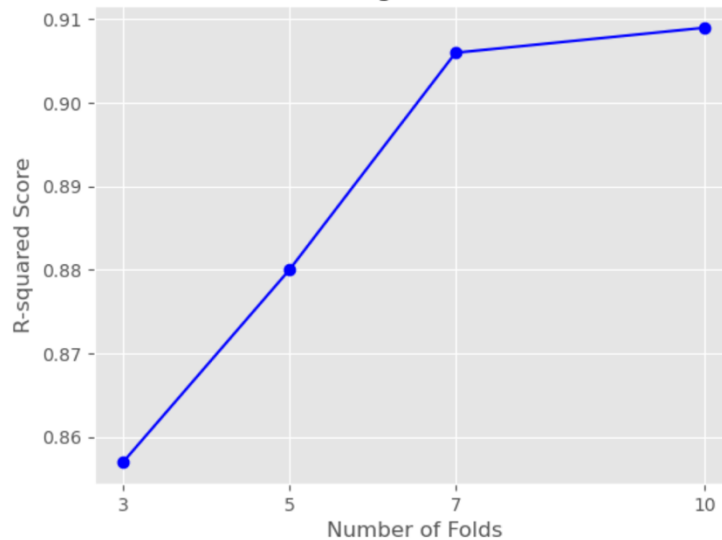
Proceeding to a 7-fold cross-validation, the best estimator maintained a consistent `max_features` parameter of 'log2'. Consequently, the R-squared score experienced a further increase to approximately 0.906. However, the mean cross-validation score on the testing set hovered around 0.770, with a standard deviation of about 0.116.

Lastly, in the 10-fold cross-validation, the best estimator retained a `max_depth` of 20 and `max_features` as 'log2', but with 200 estimators. This configuration yielded the highest R-squared score of around 0.909. Additionally, the mean cross-validation score on the testing set improved to approximately 0.781, with a standard deviation of around 0.103, showcasing slightly enhanced stability compared to the 7-fold case.

The 10-fold cross-validation scenario achieves the highest R-squared score of approximately 0.909, indicating better predictive performance compared to other scenarios (Figure 14). Despite achieving the highest R-squared score, the 10-fold cross-validation scenario also exhibits slightly higher variability in performance, as indicated by the standard deviation of the cross-validation

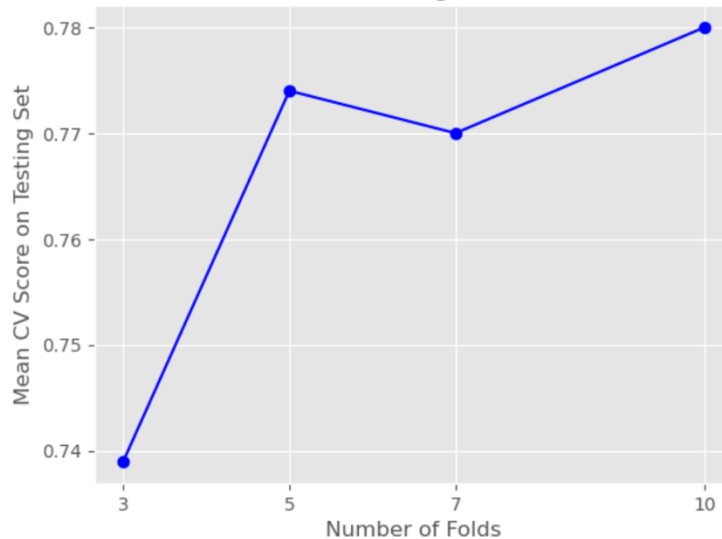
scores on the testing set (0.103). This suggests that the model's performance may vary across different folds. The mean cross-validation score provides an indication of the average performance of the model across different folds. In this case, the 10-fold cross-validation scenario also has the highest mean cross-validation score on the testing set, further supporting its superior performance on average. (Figure 15).

Best Scores for Random Forest Regression with Different Number of Folds



**Figure 14.** Best scores with different number of folds for the Random Forest model.

Mean Cross-Validation Scores on Testing Set for Random Forest Regression



**Figure 15.** The cross-validation results for the Random Forest Regression.

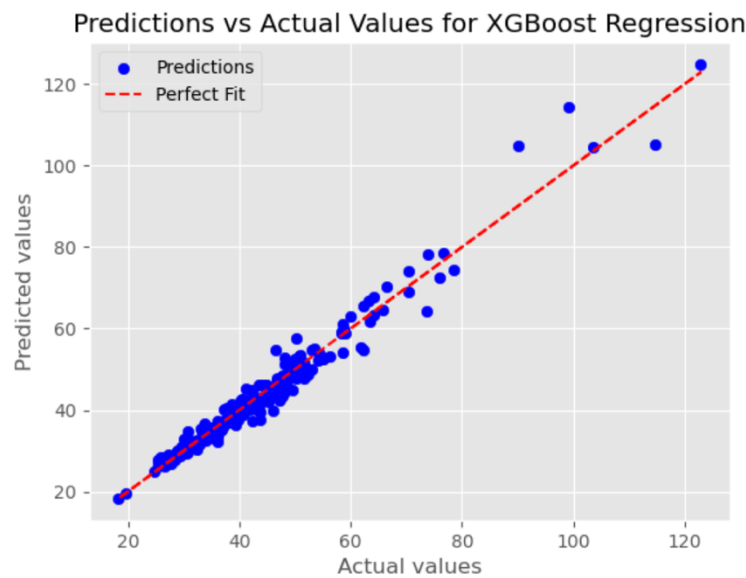
Given these considerations, the 10-fold cross-validation scenario with a Random Forest Regressor using `max_depth=20`, `max_features='log2'`, and `n_estimators=200` seems to be the

most suitable choice. It achieves the highest R-squared score and a relatively high mean cross-validation score, indicating strong predictive performance. Although there is slightly higher variability compared to other scenarios, the overall performance is superior.

## 5.5 XGBoost Regression

**XGBoost** regression model has performed exceptionally well in predicting the WQI. With an **R<sup>2</sup>** value of approximately **0.962**, the model effectively captures the variance in the target variable, demonstrating a strong fit to the dataset. Furthermore, the low **MSE** and **MAE** values, approximately **8.469** and **2.008**, respectively, highlight the model's accuracy and precision in its predictions.

Overall, these evaluation metrics indicate that the XGBoost Regression model performs very well in predicting the WQI based on the given features. As shown in Figure 16, most of the points align closely with the perfect fit line, indicating that the model's predictions are in good agreement with the actual values.



**Figure 16.** Relationship between the predicted and actual values generated by the XGBoost Regression model.

Table 2 provides an overview of the XGBoost cross-validation results, including the maximum depth, number of estimator, learning rate, the best score achieved, mean cross-validation scores on the testing sets, and the standard deviation in cross-validation scores on the testing set.

**Table 2.** XGBoost Model Cross-Validation Results.

	Cross-Validation	Max Depth	N Estimators	Learning Rate	Best Score	Mean CV Score (Testing Set)	Standard Deviation
0	3-fold	3	300	0.1	0.954	0.883	0.055
1	5-fold	3	300	0.1	0.967	0.900	0.064
2	7-fold	3	300	0.1	0.976	0.907	0.085
3	10-fold	3	300	0.1	0.973	0.926	0.063

Across all folds, the best estimator consistently utilized the following hyperparameters: 'n\_estimators': 300, 'max\_depth': 3, 'learning\_rate': 0.1. In 3-fold cross-validation, the best estimator achieved an R-squared score of approximately 0.954, indicating a good fit to the data. Similarly, in the 5-fold cross-validation scenario, the best estimator achieved an R-squared score of approximately 0.967. In the 7-fold cross-validation scenario, the best estimator achieved an even higher R-squared score of approximately 0.976, reflecting an even better fit to the data compared to previous fold scenarios. Lastly, in the 10-fold cross-validation scenario, the best estimator achieved an R-squared score of approximately 0.973.

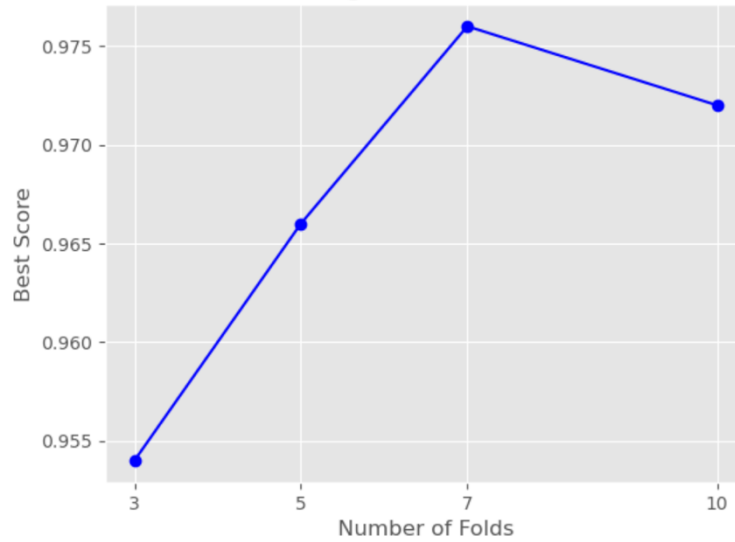
Comparing the mean cross-validation scores on the testing set across different numbers of folds, we observe a consistent trend of improved performance as the number of folds increases, indicating that the model's generalization capability enhances with a larger number of folds.

Additionally, the standard deviation in cross-validation scores on the testing set slightly increases with a higher number of folds due to the smaller size of the validation sets in each fold, leading to greater variability in model performance estimates.

Based on the mean cross-validation scores on the testing set, the 10-fold cross-validation yields the highest mean score of approximately 0.926, indicating superior generalization performance for the XGBoost Regression model.

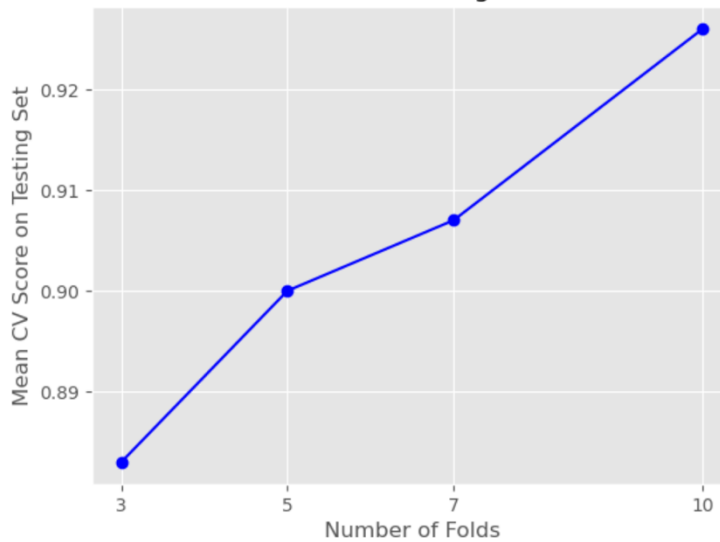
Figures 17 and 18 illustrate the best scores and mean cross-validation scores on the testing set for XGBoost Regression across different numbers of folds. The 10-fold cross-validation scenario achieves the highest mean cross-validation score on the testing set (approximately 0.926), indicating strong predictive performance. While the 7-fold cross-validation scenario also exhibits high performance, the 10-fold scenario shows slightly lower variability in performance, as indicated by the standard deviation of the cross-validation scores on the testing set. Overall, the 10-fold cross-validation scenario achieves the highest mean cross-validation score on the testing set and a relatively low standard deviation, suggesting superior overall performance compared to other scenarios.

Best Scores for XGBoost Regression with Different Number of Folds



**Figure 17.** Best scores with different number of folds for the XGBoost model.

Mean Cross-Validation Scores on Testing Set for XGBoost Regression



**Figure 18.** Mean cross-validation scores on the testing set for XGBoost regression model.

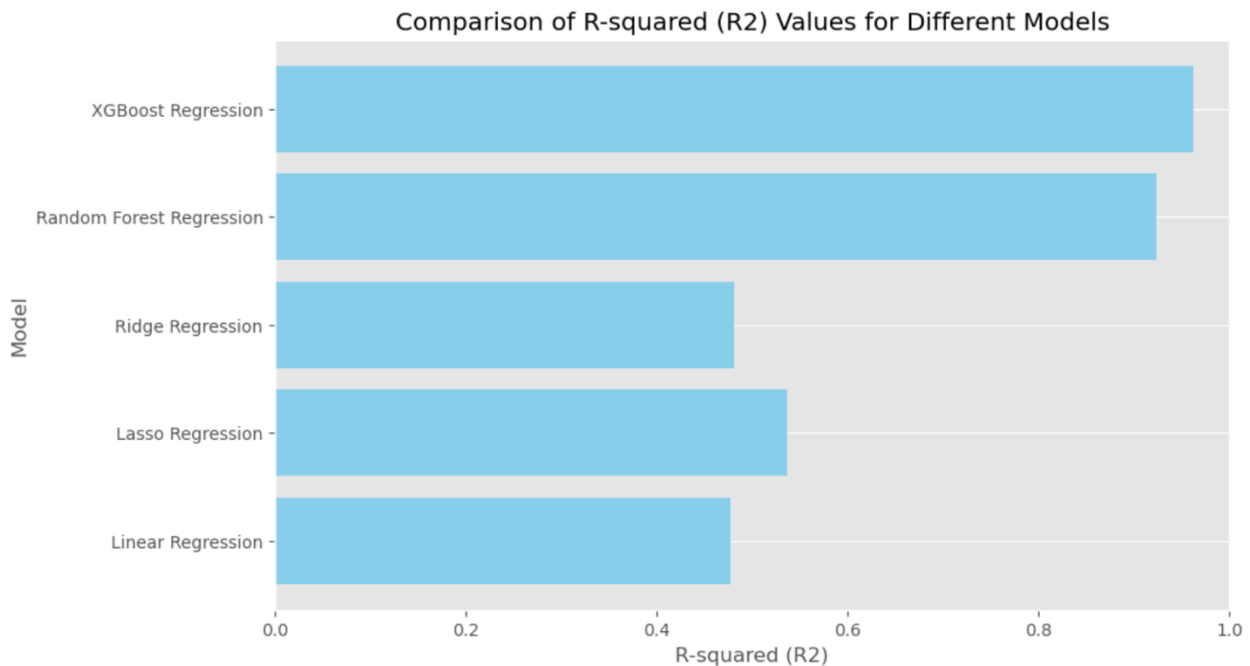
## 6 Results

The performance of each model was analyzed and compared based on evaluation metrics such as R2, MSE, MAE, and mean cross-validation scores. The strengths and weaknesses of each model was identified and determined which model performed best for predicting the

WQI. Table 1 provides the comparison of regression models and figure 19 illustrates the comparison of R2 values for different models.

**Table 3.** Comparison of regression models.

	Model	R-squared (R2)	Mean Squared Error (MSE)	Mean Absolute Error (MAE)	Mean Cross-Validation Score on Testing Set
0	Linear Regression	0.477	117.110	8.070	5-fold: 0.755
1	Lasso Regression	0.536	103.736	7.438	-
2	Ridge Regression	0.481	116.024	8.032	-
3	Random Forest Regression	0.923	17.285	2.665	10-fold: 0.781
4	XGBoost Regression	0.962	8.469	2.008	10-fold: 0.926



**Figure 19.** Comparison of R2 values for different models.

- ❑ XGBoost Regression outperforms all other models in terms of R2 (0.962) on the testing set, indicating its superior ability to explain the variance in the target variable (WQI).
- ❑ XGBoost Regression also has the lowest MSE and MAE values on the testing set compared to other models, demonstrating its accuracy in predicting the WQI.
- ❑ Among the models compared, XGBoost Regression also exhibits the highest mean cross-validation score on the testing set (0.926) using 10-fold cross-validation, indicating its robustness and consistency in performance across different data splits.
- ❑ While Random Forest Regression achieved a high R2 value (0.923) on the testing set, it has a higher MSE and MAE compared to XGBoost Regression.

- Linear Regression, Lasso Regression, and Ridge Regression have lower R-squared values and higher MSE and MAE values compared to both Random Forest Regression and XGBoost Regression, indicating poorer performance in predicting the WQI. However, Lasso Regression shows slightly better performance than Ridge Regression and Linear Regression based on the R-squared value.

## **7 Conclusion**

The modeling phase of the study aimed to develop predictive models for water quality assessment based on a range of environmental features. Through the implementation of various regression algorithms, including Linear Regression, Lasso Regression, Ridge Regression, Random Forest Regression, and XGBoost Regression, we gained valuable insights into the relationship between predictor variables and the WQI.

Our analysis revealed significant variations in the performance of the regression models. While Linear Regression, Lasso Regression, and Ridge Regression demonstrated moderate predictive capabilities, Random Forest Regression and XGBoost Regression outperformed them significantly. Specifically, XGBoost Regression emerged as the top-performing model, achieving an impressive  $R^2$  value of 0.962 on the testing set, along with the lowest MSE and MAE values.

Our study showed the importance of selecting appropriate features, models, and evaluation metrics for accurate water quality prediction. Moreover, we identified key factors influencing water quality prediction, providing valuable insights for future research and decision-making processes.

However, our study has some limitations. The data we used might not be perfect, and the assumptions we made during modeling could affect the accuracy of our results. Also, there might be other factors affecting water quality that we didn't consider in our analysis.

## **8 Recommendations**

Based on our findings, there are several promising directions for future research. Firstly, there's room to explore feature engineering further by adding more environmental, geographical, and human-related factors. This exploration could significantly enhance the predictive power of our models by uncovering hidden patterns and relationships within the data.

Furthermore, investigating seasonal variations and long-term trends in water quality could provide valuable insights into how environmental factors impact water quality over time. Utilizing time-series modeling techniques would allow for a comprehensive understanding of these temporal patterns. Employing spatial analysis techniques, such as Geographic Information System (GIS) tools, would enable the exploration of spatial patterns in water quality, identifying areas of concern and informing targeted interventions and management strategies.

Additionally, exploring the application of deep learning methods, such as neural networks, for water quality prediction could yield significant improvements in predictive accuracy. These models excel at capturing complex relationships in data and may offer novel insights into water quality dynamics. Lastly, validating our models in real-world scenarios through field studies is essential. This ensures their practical usefulness and reliability for decision-makers.



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