MACHINE LEARNING FOR WATER QUALITY INDEX PREDICTION: A REVIEW ON TECHNIQUES, CHALLENGES AND APPLICATIONS

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ABSTRACT

Water Quality assessment is crucial for maintaining ecological balance and community health. The Water Quality Index (WQI) is a simplified value derived from the analysis of the chemical, physical, and biological parameters of water. Recently, artificial intelligence and machine learning approaches have proven to be promising techniques for predicting of WQI. This study examines different machine learning techniques used to predict the Water Quality Index and highlights their ability to surpass traditional statistical methods. This study examines different machine learning techniques used to predict the Water Quality Index and highlights their ability to surpass traditional statistical methods. This study examines different machine learning techniques used to predict the Water Quality Index and highlights their ability to surpass traditional statistical methods. Techniques such as Random Forest (RF), Support Vector Machines (SVM), and Artificial Neural Networks (ANN) are highlighted for their robust performance in analysing complex and nonlinear relationships within water quality datasets. This review underscores the promise of artificial intelligence and machine learning in evaluating water quality. It also points out existing research gaps and suggests future paths to connect water resource management with technological advancements.

INTRODUCTION

Environmental processes in a given area are influenced by two key determinants that affect surface water quality: naturally occurring factors and those resulting from human intervention. Natural elements include precipitation intensity, soil degradation, and plant life, while human-related factors encompass household and industrial waste discharges, as well as agricultural drainage. Urban and industrial wastewater releases constitute a steady source of contamination, whereas surface water runoff is affected by weather-related variables. When pollutants enter ecosystems like lakes, rivers, or estuaries, they trigger physical, chemical, and biological processes, resulting in specific pollutant concentrations within these water bodies. Effective long-term management of water quality necessitates a comprehensive understanding of these physical, chemical, and biological characteristics. Consequently, monitoring water bodies is crucial for informed management and development of water resources. To capture spatial-temporal variations in water quality, including seasonal changes, a continuous monitoring program is essential. Such programs generate extensive data matrices that require interpretation through various statistical methods to accurately assess the ecological status and water quality of the studied water body.

To effectively communicate water quality information to the public, developing an indicator is crucial. This indicator should express overall quality at a specific location and time. The

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purpose of a water quality index (WQI) is to distil information from multiple water quality parameters into a single numerical value through the use of a mathematical equation. This approach allows for the synthesis of diverse data points into one comprehensive metric. WQIs can be used to assess the health of any water body and have been developed and applied in various surface and groundwater ecosystems worldwide. Comprehensive reviews of WQIs can be found in Bharti and Katyal (2011), Tyagi et al. (2013), and Sutadian et al. (2016).

Environmental monitoring has been revolutionized by the application of machine learning algorithms. These advanced computational techniques excel in processing vast amounts of environmental data, uncovering subtle patterns and relationships that traditional analytical methods might overlook. By leveraging machine learning, researchers can gain deeper insights into environmental systems, enhancing their ability to detect and interpret complex ecological phenomena. (Shalu & Singh, 2023). These techniques have been successfully applied to various aspects of environmental sustainability, including biodiversity, energy, transportation, and water management (Nti et al., 2022). Furthermore, the combination of AI and machine learning technologies with remote sensing data and satellite imagery has created new opportunities for environmental evaluation and surveillance. These cutting-edge technologies allow for the extensive acquisition of significant data from a wide range of spatially referenced resources (Himeur et al., 2022). From biodiversity research to water resource conservation, energy management, and transportation, AI and ML are providing innovative solutions to complex environmental challenges (Himeur et al., 2022; Nti et al., 2022). This paper seeks to examine the potential applications of these computational techniques within the field of water quality assessment.

WATER QUALITY INDEX (WQI) AND ITS PARAMETERS

Water Quality Index (WQI) serves as a statistical method for simplifying, communicating and interpreting complex water quality data by converting it into a single numerical value (Rubio-Arias et al., 2012). It provides an overall assessment of water quality status, helping in the selection of appropriate treatment techniques and communicating information to the public and decision-makers (Tyagi et al., 2020). The development of Water Quality Index (WQI) models generally encompasses four key steps: choosing relevant water quality parameters, creating sub-indices for each selected parameter, determining the weighting values for these parameters, and combining the sub-indices to derive the final comprehensive index. (Uddin et al., 2020). Some indices also consider additional parameters such as temperature, electrical conductivity, and chemical oxygen demand (Kannel et al., 2007; Othman et al., 2020). However, the absence of a globally accepted composite index of water quality has led to the development of various country-specific indices (Tyagi et al., 2020).

KEY PHYSICOCHEMICAL AND BIOLOGICAL PARAMETERS Water quality assessments typically measure several essential physicochemical and biological factors. These include, but are not limited to, pH levels, the amount of oxygen dissolved in water (DO), biochemical oxygen demand (BOD), the total quantity of dissolved solids (TDS), and water clarity or turbidity. pH is an important indicator of water quality, with most studies reporting slightly acidic to neutral values ranging from 5.05 to 7.0 (Chinedu & Nwinyi, 2011; Leong et al., 2018). Dissolved oxygen (DO) is crucial for aquatic life and tends to decrease downstream as pollution increases (Ahipathy & Puttaiah, 2006; Melaku et al., 2007). BOD and chemical oxygen demand (COD) are measures of organic pollution, with higher values indicating more contamination (Chinedu & Nwinyi, 2011; Kannan et al., 2006). TDS represents the concentration of dissolved substances and is often correlated with electrical conductivity (EC)

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(Shroff et al., 2015). Turbidity, which measures water clarity, can be significantly reduced through treatment processes like electrocoagulation (Kannan et al., 2006). Interestingly, some studies found correlations between these parameters. For instance, EC was found to be significantly correlated with eight out of seventeen water quality parameters in one study (Shroff et al., 2015). Additionally, seasonal variations were observed in several physicochemical parameters, except for calcium, potassium, and total alkalinity in some cases (Zafar & Kumari, 2024).

TRADITIONAL METHODS OF WQI CALCULATION

Method	Description	Key Features
Weighted Arithmetic Method (Horton, 1965)	The first WQI method, developed by Horton. Uses a weighted sum of normalized water quality parameters.	Assigns weights based on the significance of parameters. Easily interpretable.
WQI by National Sanitation Foundation (NSFWQI) (Brown et al., 1970)	Developed in USA, based on Delphi technique and expert opinion. Uses a combination of additive and multiplicative methods.	Standardized method used globally. Based on expert consensus.
Munich Method (Liebman, 1969)	Uses color-coded maps for water quality assessment in Bavaria, Germany.	Visual representation of water quality. Subjective weighting of parameters.
River Pollution Index (RPI) (McDuffie & Haney, 1973)	Uses eight pollutant variables, such as BOD, coliform count, and oxygen deficit.	Focuses on river pollution. Simple to apply.
Recreational Water Quality Index (Walski & Parker, 1974)	Designed for assessing water quality for recreational uses. Uses geometric mean of selected parameters.	Specific to recreational water quality.Parameters include turbidity, pH, and coliform count.
Scottish Water Quality Index (SRDD WQI) (SRDD, 1976)	Developed using Delphi method; later adapted for different river basins worldwide.	Used internationally in Scotland, Thailand, Spain, and Portugal.
Ross Index (Ross, 1977)	Developed for the Clyde catchment in Britain; evolved into a weighted additive model.	Includes separate indices for general water quality, toxicity, potable supply, and sapidity.
Bascaron Index (Bascaron, 1979)	Initially for general water quality but later adapted for aquaculture.	Flexible in parameter selection. - Used in Spain, Latin America.
Oregon Water Quality Index (OWQI) (Dunette, 1979; Cude, 2001)	Based on harmonic averaging of selected parameters. Used for recreational water quality.	Focused on Oregon’s rivers. Adapted for Idaho rivers.
Index of Biotic Integrity (IBI) (Karr, 1981)	Biological assessment using fish communities to determine water quality.	Commonly used in ecological studies.
British Columbia Water Quality Index (BCWQI) (1990s)	Compares measured parameters with regulatory limits.	Used in Canada. - Does not show trends unless deviation is significant.

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Water Quality Index (WQI) developed by the Canadian Council of Ministers of the Environment (CCME) in 2001	A flexible, standardized index used in Canada and globally.	Considers multiple water uses. - Overestimates certain factors.
Dalmatian Index (Stambuk–Gilianovic, 1999)	Arithmetic index using 9 parameters to assess general water quality in Serbia.	Used for large-scale water quality assessment.
Universal Water Quality Index (UWQI) (Boyacioglu, 2007)	A simple WQI for drinking water assessment.	Focused on UN Millennium Development Goals.
Global Drinking Water Quality Index (GDWQI) (Rickwood & Carr, 2009)	Based on CCME WQI, developed for global drinking water assessment.	Used internationally.
Overall Index of Pollution (OIP) (Sargaonkar & Deshpande, 2003)	Indian WQI that classifies water based on Indian and WHO standards.	Widely used in India.

MACHINE LEARNING TECHNIQUES FOR WQI PREDICTION

The ability of machine learning to predict water quality is particularly effective due to its capacity to uncover potentially intricate relationships between variables and their anticipated outcomes.

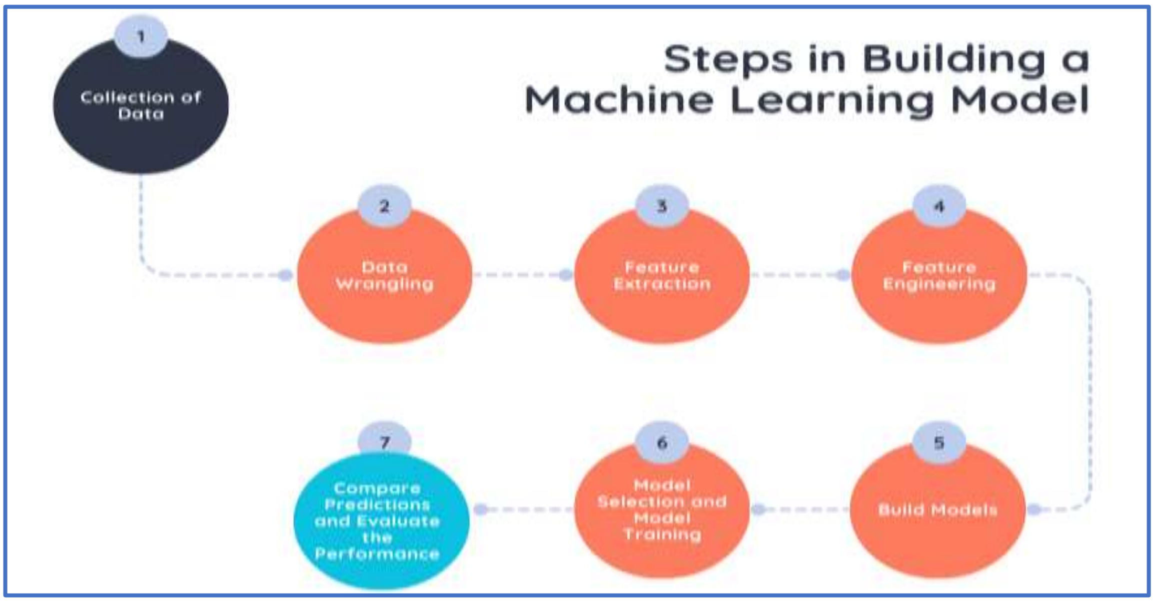

Figure 1. Stages involved in developing a model using machine learning.

Machine learning offers a powerful toolkit for predicting water quality, encompassing various techniques suitable for different scenarios and data characteristics. Here's a breakdown of some common approaches:

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SUPERVISED LEARNING Supervised learning methods train models on labeled datasets, learning the relationship between input features (e.g., temperature, pH, dissolved oxygen) and target variables (e.g., Water Quality Index, presence of specific pollutants).

1. Regression models predict continuous water quality parameters. Common algorithms include:
   - Multivariate Linear Regression**:** A simple yet effective method for establishing linear relationships between multiple input features and a target variable (Abyaneh, 2014). Suitable for datasets with linear dependencies.

   - Support Vector Regression: Effective for non-linear relationships, the objective of SVR is to identify the optimal hyperplane that divides data points while reducing the error in predictions to a minimum.(Yan et al., 2019).
   - Polynomial Regression: Models non-linear relationships using polynomial functions (Ahmed et al., 2019). Suitable when data exhibits curvilinear patterns.

2. Classification models predict categorical water quality variables (e.g., water quality classes). Common algorithms include:
   - Artificial Neural Networks: Highly adaptable models capable of learning complex non-linear relationships (Abyaneh, 2014). Effective for large datasets and intricate patterns.
   - Decision Trees: Develop a hierarchical system (tree-like structure) for organizing information through a sequence of choicess (Nayan et al., 2021). Easy to interpret and visualize.
   - Gradient Boosting: A technique that integrates several weak predictive models, usually decision trees, to produce a robust and accurate predictive system(Ahmed et al., 2019). Known for high accuracy and robustness.

UNSUPERVISED LEARNING Unsupervised learning methods analyze unlabeled datasets to discover underlying patterns and structures. Data points with similar attributes are grouped together using clustering algorithms. Some commonly used techniques include:

- K-means clustering: Divides data into k clusters by measuring the distance between data points and cluster centers (Azhar et al., 2015). Useful for identifying distinct water quality regimes.
- Hierarchical clustering: Builds a hierarchy of clusters, ranging from individual data points to a single all-encompassing cluster (Azhar et al., 2015). Useful for exploring relationships between different water quality states.

TIME SERIES ANALYSIS Time series analysis techniques are specifically designed for sequential data, capturing temporal dependencies in water quality parameters.

- Long Short-Term Memory Networks: A recurrent neural network designed to recognize and learn patterns in sequential data over extended periods (Yan et al., 2019; Yang & Liu, 2021). Capable of forecasting future water quality patterns by analyzing historical data trends.

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Table 2. Machine Learning Approaches for WQI Prediction

Category of Machine Learning Approach	Key findings	References	Limitations/ Weakness
Supervised Learning Approaches	Random Forest (RF) is a top performer, optimized with feature selection. - Extra Tree Regression (ETR) provides high accuracy. - Neural networks (MLP-NN, DNN) outperform other models in specific contexts. - Feature selection significantly impacts model performance. - Multiple Linear Regression (MLR) achieved comparable accuracy with fewer parameters.	Asadollah et al. (2020), Raheja et al. (2021), Suwadi et al. (2022), Castillo et al. (2022), Aish et al. (2023), Othman et al. (2020), Mo et al. (2024), Lap et al. (2023)	- Requires labeled training data, which may not always be available. - Performance highly depends on feature selection. - Struggles with complex, nonlinear relationships in water quality data.
Unsupervised Learning Approaches	- Used mainly for anomaly detection (OneClassSVM, LOF, IF, EE). - Comparable to or better than supervised methods in anomaly detection. - Limited research on unsupervised learning for direct WQI prediction. - Potential for hybrid models integrating supervised and unsupervised techniques.	Suwadi et al. (2022), Shriram & Sivasankar (2019), Uddin et al. (2020), Hoseinzadeh et al. (2014), Kannel et al. (2007),	Limited success in direct WQI prediction. - Difficult to interpret results compared to supervised methods. - Performance depends on the quality and variability of the dataset.
Deep Learning Models	CNNs, GRUs, and BiLSTMs show high accuracy for WQI prediction. - Stacking models outperform standalone CNNs. - Some traditional ML models (ETR, XGBoost) match deep learning models in certain cases. - Explainable AI techniques (SHAP values) provide insights for water management. - LSTMs perform well for time-series WQI prediction in river water.	Alshehri & Rahman (2023), Othman et al. (2020), Farzana et al. (2023), , Khozani et al. (2022), Mo et al. (2024), Asadollah et al. (2020)	- Requires large amounts of training data. - Computationally expensive and requires high-performance hardware. - Prone to overfitting, especially with small datasets.

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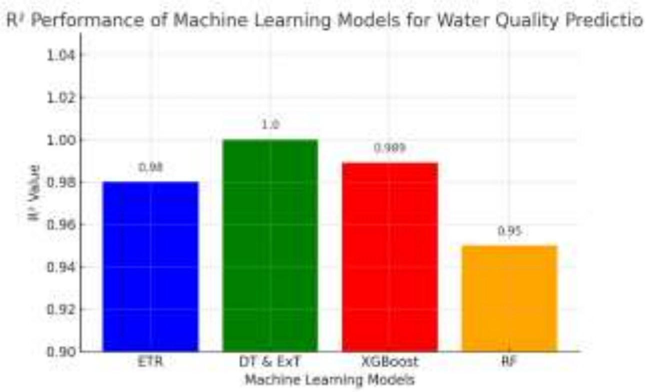
MODEL EVALUATION AND PERFORMANCE METRICS

Machine learning models for water quality prediction are evaluated using various performance metrics to assess their accuracy and reliability. Common metrics include coefficient of determination (R^2), root mean square error (RMSE), mean absolute error (MAE), and F1-score (Khoi et al., 2022; Mohseni et al., 2024; Uddin et al., 2022). Machine learning models have shown great potential in predicting water quality indices with high accuracy. Tree-based models and ensemble methods like ETR, XGBoost, and Random Forest consistently perform well across multiple studies. However, the choice of the best model may differ based on the particular water quality indicators and the characteristics of the dataset. Researchers should consider evaluating multiple models and metrics to determine the most suitable approach for their specific water quality prediction tasks.

Table 3. Performance of Machine Learning Models for Water Quality Prediction

Model	R	RMSE	MAE	Performance Insights	References
Extra Tree Regression (ETR)	0.98	2.99	N/A	High accuracy with all ten input variables, widely used for WQI prediction.	Asadollah et al. (2020)
Decision Tree (DT) & Extra Tree (ExT)	1.0	0.0	0.0	Achieved perfect performance metrics in coastal water quality assessment.	Uddin et al. (2022)
Extreme Gradient Boosting (XGBoost)	0.989	0.107	N/A	Outperformed other models in some studies, highlighting dataset dependency.	Khoi et al. (2022)
Random Forest (RF)	High	Varies	Varies	Consistently strong performer across multiple studies.	Uddin et al. (2022), Mohseni et al. (2024)

Here is a bar chart visualizing the R^2 performance of different machine learning models for water quality prediction.



1 Performance of various ML models for Water Quality Prediction

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CHALLENGES IN MACHINE LEARNING-BASED WQI PREDICTION

Predicting the Water Quality Index using machine learning models comes with several challenges. Data scarcity and quality issues are major hurdles. Traditional assessment methods are often expensive and time-consuming, hindering real-time monitoring (Uddin et al., 2020). Limited data can negatively impact the performance of even complex models like Convolutional Neural Networks (Chen et al., 2019). Another challenge is generalizing models across diverse water bodies and locations. Water quality is influenced by local environmental factors, pollution sources, and seasonal changes (Uddin et al., 2020). Therefore, models need to adapt to these variations to be effective (Wang et al., 2017). Researchers are exploring various strategies to overcome these challenges, such as feature selection to optimize data collection and model training, and ensemble methods or hybrid models to improve prediction accuracy.

CONCLUSION

The selection of machine learning algorithms depends on the water quality parameters being simulated. For dissolved oxygen prediction, Random Forest slightly outperforms Support Vector Machine. Multiple water quality parameters can be predicted using Support Vector Regression, Extreme Gradient Boost, and Random Forest, with ensemble machine learning models also showing promise. Various models, including Random Forests, Extreme Gradient Boosting, Convolutional Neural Network, Multi-layer Perceptron and Short-term Memory, have demonstrated good efficacy in predicting WQI. The Random Forest algorithm is remarkably capable in identifying crucial water quality indicators, while the Deep Neural Network algorithm excels in predicting specific subsets.

This review provides a thorough overview of how machine learning is being used to predict water quality. While many models have been developed, finding a universally "best" approach is difficult, as model performance varies depending on the specific water quality parameters and the region being studied. Improving prediction accuracy requires more data (Yang, 2023), potentially using remote sensing and other innovative data acquisition methods, and better handling of missing data through techniques like interpolation (Willard et al., 2023). This review serves as a valuable resource for anyone interested in the complexities and advancements of this field.

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