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**Review Article**

# MACHINE LEARNING-BASED PREDICTION OF WATER QUALITY USING PHYSICOCHEMICAL AND ENVIRONMENTAL INDICATORS

**Dr. Rakhi Dua**

Assistant Professor, K. R Mangalam University, Email: rakhi.dua@krmangalam.edu.in

***Abstract***

*Reliable prediction of water quality can strengthen environmental monitoring by integrating conventional measurements with data-driven analytical approaches. This study evaluated the capacity of physicochemical, environmental, spatial, and hydrological indicators to predict an integrated water-quality score using machine-learning regression. The analysis included 36 complete observations from Anuppur, Dindori, and Jabalpur and incorporated indicators of oxygen conditions, organic loading, nutrients, ionic composition, microbiological contamination, rainfall, water level, season, and location. Four algorithms—Ridge Regression, Random Forest, Gradient Boosting, and Decision Tree Regression—were evaluated using six-fold cross-validation. Distinct spatial patterns were observed, with Jabalpur recording the highest mean water-quality impairment score and Anuppur the lowest. Total coliform, phosphate, BOD, conductivity, dissolved solids, and COD showed strong positive associations with the integrated outcome. Ridge Regression achieved the strongest overall predictive performance ($R^2 = 0.603$; RMSE = 6.98; MAE = 5.01), while Random Forest produced the lowest MAE (4.93). The findings demonstrate that a parsimonious machine-learning framework can capture meaningful water-quality variability from multidimensional environmental measurements. Although the limited sample size constrains generalizability, the approach provides a practical basis for identifying influential indicators and supporting targeted water-quality monitoring.*

**Keywords:** Water quality, Machine learning, Physicochemical indicators, Environmental monitoring, Predictive modelling

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## Introduction

Fresh water is essential for people, farming activities, industrial development, the functioning of ecosystems, and social and economic stability. The demand for water has increased, populations have grown, climate variability has been felt, and the availability of fresh water in the world is unevenly distributed, which has led to a greater awareness of water availability and quality issues globally (Mishra, 2023). Additionally, ecological and economic values of freshwater systems exist that rely on the physical, chemical and biological integrity of these systems. The need for effective monitoring, management and conservation strategies which can help the sustainable use of freshwater resources has therefore increased due to increased exposure to multiple stressors (Bănăduc et al., 2022).

Water quality in the surface water is the result of natural processes and human activities. Aquatic conditions are altered by the interaction of weathering, erosion, precipitation, the hydrological fluctuations and the catchment characteristics, along with agricultural runoff, urban wastewater, and industrial discharge as well as land use change (Akhtar et al., 2021). These influences can change the nutrient levels, organic material, ionic composition, suspended material and oxygen availability. Thus, the water quality assessment is based on various physicochemical parameters including pH, temperature, turbidity, conductivity, dissolved solids, dissolved oxygen, biochemical oxygen demand (BOD) and chemical oxygen demand (COD), nutrients, alkalinity and hardness. A water-quality index that combines several parameters can give a more readily interpretable value for the overall water quality than individual values (Nayar, 2020). However, careful selection of parameters that represent pollution pressure and physical and chemical changes of water is required for reliable assessment (Misman et al., 2023).

Rarely water-quality conditions are homogeneous (the same) over space or time. These rainfall, water level, season, catchment processes, and sampling location differences may alter pollutant transport, dilution, nutrient loadings, sediment movement, and biological activity. The significant temporal and spatial variations have been reported on river networks where the environmental factors influence water-quality characteristics (Zhu et al., 2022). Water quality patterns and the relationship between water quality and environmental flows also can be affected by hydrological conditions. (Zhao et al., 2020). The movement of nutrients, sediments, and contaminants to freshwater systems from land use is also influenced by seasonal rainfall and the surrounding land use characteristics (Umwali et al., 2021). The addition of environmental and hydrological data with traditional physicochemical data might accordingly enhance the understanding of the variability of water quality.

Traditional monitoring methods offer valuable data and require field sampling, lab measurement, and periodic observations. The frequency of monitoring is limited by these requirements and rapid changes in conditions can not be identified in real time. The development and improvement of water quality monitoring technologies have gradually moved towards a more automated and computation-based system and has become a complement to traditional water quality monitoring (Ahmed et al., 2020). Online sensors are able to detect contamination events and can consider the normal fluctuations in water properties routinely monitored (Koppanen et al., 2022). In order to address the challenges of fragmented observations, long-term monitoring strategies are now highlighting the need for continuous measurements, advanced sensing technologies, and integrated analytical systems (Huang et al., 2022). Conventional assessment, however, is still valuable as it offers standardized assessments that are essential for the advanced analytical methods (Babatunde, 2024).

A trend towards virtual and data-driven environmental sensing for estimation is also emerging as environmental data becomes available. Virtual sensing can leverage relationships among variables measured to estimate water-quality conditions and increase the analytical value of monitoring networks (Paepae et al., 2021). Machine learning is especially relevant as it can simultaneously assess multiple predictors and can detect relationships that are not easily recognized when using traditional univariate assessment methods. Recently, regression, decision-tree, ensemble, and other algorithms have been used for water-quality assessment, prediction, and identification of the factors affecting the water quality (Zhu et al., 2022).

Although these advances have been made, there is still a significant lack of linkage between physicochemical indicators and environmental, spatial, seasonal and hydrological information in an interpretable predictive framework. Many evaluations focus on certain water-quality parameters, and very complex machine-learning applications may not be warranted for relatively small environmental monitoring data sets. A pragmatically simple modelling approach, using traditional water-quality data along with environmental predictors might yield useful predictive information and remain interpretable and relevant. Based on this, the goals of this study were formulated as follows:

- To characterize physicochemical, spatial, and seasonal variability in water-quality conditions.
- To develop and compare machine-learning models for predicting integrated water quality.
- To identify the physicochemical and environmental indicators contributing most strongly to water-quality prediction.

## 2. Materials and Methods

### 2.1 Study Design and Data Source

A quantitative secondary-data design was applied for water quality evaluation and construction of water quality predictive models using the values of physicochemical and environmental indicators (Dilip, 2024). This data set had 36 complete observations from Anuppur, Dindori and Jabalpur and there were no missing observations in the analytical sample.

### 2.2 Water-Quality and Environmental Indicators

The parameters measured in the data set were temperature, turbidity, pH, conductivity, dissolved solids, dissolved oxygen, BOD, COD, nutrients, major ions, hardness, alkalinity and total coliform. Environmental and spatiotemporal variables were rainfall, water level, season, nature of the monitoring location, latitude, longitude, and sampling period. These variables measured chemical, physical, microbiological and hydrological aspects of surface-water quality. Data Pre-processing and Water-Quality Score.

### 2.3 Data Preprocessing and Water-Quality Score

Continuous variables were converted to numbers and categorical variables were coded when necessary. A composite water-quality rating was derived from selected indicators of water quality that include both physical/chemical and microbiological parameters, and higher values indicate higher water-quality degradation. The variables were deconstructed to reduce the leakage of information when they are model predictors.

### 2.4 Statistical Analysis

All analyses were performed in Python with the use of Pandas, NumPy, SciPy and scikit-learn. For continuous variables, the mean, standard deviation, minimum and maximum values were used. Monitoring locations and seasons were compared to determine spatial and seasonal patterns. To determine associations between the measured indicators and the integrated water-quality score, Spearman's rank correlation was used. A p value of $< 0.05$ was considered statistically significant.

### 2.5 Machine-Learning Modelling

Four regression models (Ridge Regression, Random Forest Regression, Gradient Boosting Regression and Decision Tree Regression) were built to predict a continuous water-quality score. Physicochemical, environmental, spatial and hydrological variables not directly used in the construction of the scores were used as predictors. All continuous variables were standardized as needed and categorical variables were coded prior to modelling.

### 2.6 Model Validation and Evaluation

Due to the small number of observations 6-fold cross validation was used so that each observation could be used in the out-of-sample assessment. The coefficient of determination ($R^2$), root mean squared error (RMSE) and mean absolute error (MAE) were used to evaluate the performance of the models. The obtained $R^2$ values and minimization of the error showed better predictive performance. The comparative performance estimates that are reported for the four models were produced by these procedures.

**2.7 Model Interpretation and Visualization**

The model with the best performance was chosen based on the cross-validated performance metrics. Predictive agreement was assessed by comparing the observed and predicted water-quality scores. Spatial and temporal visualizations of data were also created to help describe the spatial and temporal changes in monitoring locations, and to aid in interpretation of the influence of physical and chemical characteristics and environmental conditions on water quality.

**3. Results**

The data analysed were 36 full observations of Anuppur, Dindori and Jabalpur. The overall water quality score based on the basic physicochemical and microbiological parameters ranged between 12.41 and 57.23 with an average of 28.02 ± 11.24. The higher the score, the more the water quality was impaired, relative to others.

**3.1 Physicochemical and Environmental Characteristics**

The data in Table 1 indicate that there is considerable variation between the measured indicators. Mean pH was 7.64 ± 0.33, while dissolved oxygen averaged 7.46 ± 0.61 mg/L. BOD and COD averaged 1.21 ± 0.62 and 8.75 ± 5.57 mg/L, respectively. The conductivity values were between 196.30 and 829.00 µS/cm, which revealed high ionic variation. There was also a considerable difference in the total coliform, ranging from 1.80 to 63.00. Environmental conditions were heterogeneous, the rainfall varied from 0.43 to 293.53 mm and the water level from 298.29 to 663.56 m.

**Table 1. Descriptive Statistics of Major Physicochemical and Environmental Water-Quality Indicators**

| Indicator | Mean | SD | Minimum | Maximum |
|---|---|---|---|---|
| Temperature (°C) | 20.69 | 9.76 | 2.00 | 29.50 |
| Turbidity | 4.25 | 2.87 | 1.00 | 16.30 |
| pH | 7.64 | 0.33 | 6.67 | 8.51 |
| Conductivity (µS/cm) | 281.71 | 111.21 | 196.30 | 829.00 |
| Dissolved solids (mg/L) | 204.89 | 47.74 | 159.00 | 428.00 |
| Dissolved oxygen (mg/L) | 7.46 | 0.61 | 5.70 | 8.50 |
| BOD (mg/L) | 1.21 | 0.62 | 0.10 | 2.60 |
| COD (mg/L) | 8.75 | 5.57 | 2.00 | 24.00 |
| Nitrate nitrogen (mg/L) | 0.42 | 0.35 | 0.14 | 1.50 |
| Phosphate (mg/L) | 0.08 | 0.16 | 0.00 | 0.60 |
| Total coliform | 29.03 | 20.14 | 1.80 | 63.00 |
| Rainfall (mm) | 61.32 | 76.99 | 0.43 | 293.53 |

3.2 Spatial and Seasonal Variation

Spacial differences were evident. As can be seen in Figure 1, the mean integrated water-quality score (37.78) and COD concentration (14.33 mg/L) were the highest in Jabalpur than in other stations, and COD concentration was lowest in Anuppur when compared with other stations, whereas BOD was lower in Anuppur. The mean turbidity (5.79), dissolved oxygen (7.99 mg/L), and rainfall (97.79 mm) were highest at Dindori, thus presenting unique water-quality characteristics of the monitoring sites.

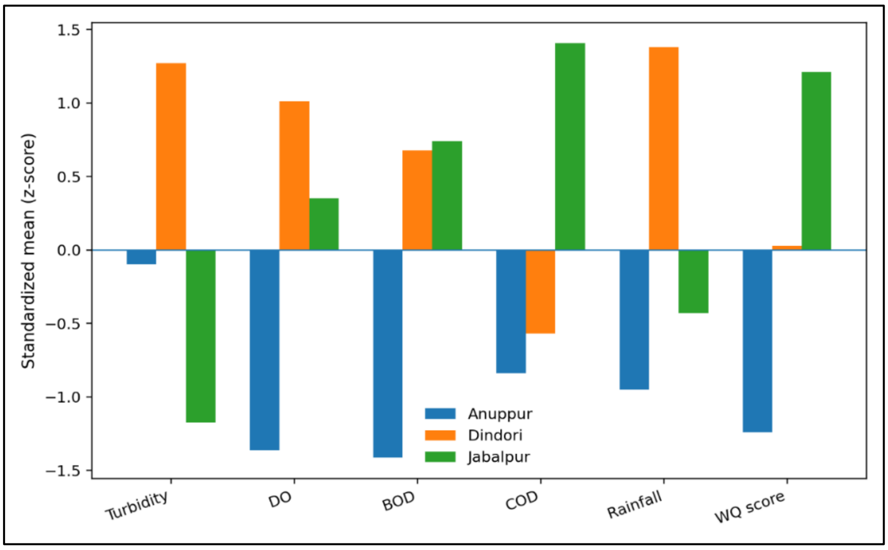


**Figure 1. Spatial Profiles of Major Physicochemical, Environmental, and Integrated Water-Quality Indicators**

As per Table 2, the mean water-quality score for monsoon season was recorded as 30.96 and the turbidity recorded as 5.61 while summer and winter recorded a score of 25.73 and 26.15 respectively. Lowest rainfall for the winter had the highest mean COD (10.02 mg/L) indicating seasonal differences for each water-quality parameter.

**Table 2. Spatial and Seasonal Variation in Selected Water-Quality Indicators**

| Group | Turbidity | DO (mg/L) | BOD (mg/L) | COD (mg/L) | Rainfall (mm) | Water-Quality Score |
|---|---|---|---|---|---|---|
| Anuppur | 4.13 | 6.73 | 0.65 | 5.43 | 36.21 | 18.03 |
| Dindori | 5.79 | 7.99 | 1.48 | 6.50 | 97.79 | 28.24 |
| Jabalpur | 2.83 | 7.64 | 1.51 | 14.33 | 49.96 | 37.78 |
| Summer | 3.53 | 7.28 | 1.21 | 7.51 | 83.03 | 25.73 |
| Monsoon | 5.61 | 7.47 | 1.13 | 8.99 | 79.29 | 30.96 |
| Winter | 2.97 | 7.68 | 1.37 | 10.02 | 2.42 | 26.15 |

Although the seasonal mean is higher for the monsoon period, the amount of overlap in the water-quality scores between the two seasons is large (see Figure 2). This shows that one seasonality category was not the only determining factor for this variation and that a number of physicochemical and environmental factors acted in conjunction.

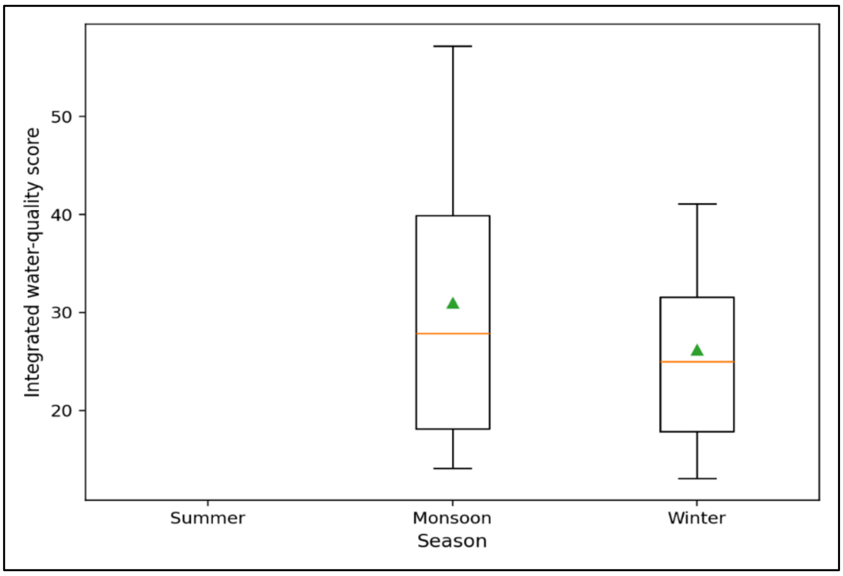


**Figure 2. Seasonal Distribution of the Integrated Water-Quality Score**

### 3.3 Associations and Machine-Learning Performance

Strong positive correlations with the integrated score were observed for total coliform (ρ = 0.836, $p < 0.001$), phosphate (ρ = 0.786, $p < 0.001$), BOD (ρ = 0.773, $p < 0.001$), conductivity (ρ = 0.699, $p < 0.001$), dissolved solids (ρ = 0.692, $p < 0.001$), and COD (ρ = 0.630, $p < 0.001$). There was an inverse correlation between the score and temperature (ρ = −0.514, p = 0.001), and no independent association between rainfall and the score (ρ = 0.102, p = 0.555).

As listed in Table 3, Ridge Regression got the best cross validated performance ($R^2 = 0.603$; RMSE = 6.98; MAE = 5.01). Random Forest was also performing in a similar manner (R2 = 0.575) and gave the least value for MAE (4.93). Gradient Boosting and Decision Tree had lower $R^2$ values (0.518 and 0.333 respectively).

**Table 3. Cross-Validated Performance of Machine-Learning Models for Water-Quality Prediction**

| Model | $R^2$ | RMSE | MAE | Rank |
|---|---|---|---|---|
| Ridge Regression | 0.603 | 6.98 | 5.01 | 1 |
| Random Forest | 0.575 | 7.22 | 4.93 | 2 |
| Gradient Boosting | 0.518 | 7.69 | 5.23 | 3 |
| Decision Tree | 0.333 | 9.05 | 6.32 | 4 |

Generally, the water-quality scores observed were fairly consistent with the Ridge Regression predictions, with the differences growing larger at the extremes, as illustrated in Figure 3. The cross-validated $R^2$ of 0.603 suggests that the model accounted for a significant amount of the water-quality variability but that a large portion of the differences in water quality remained unexplained.

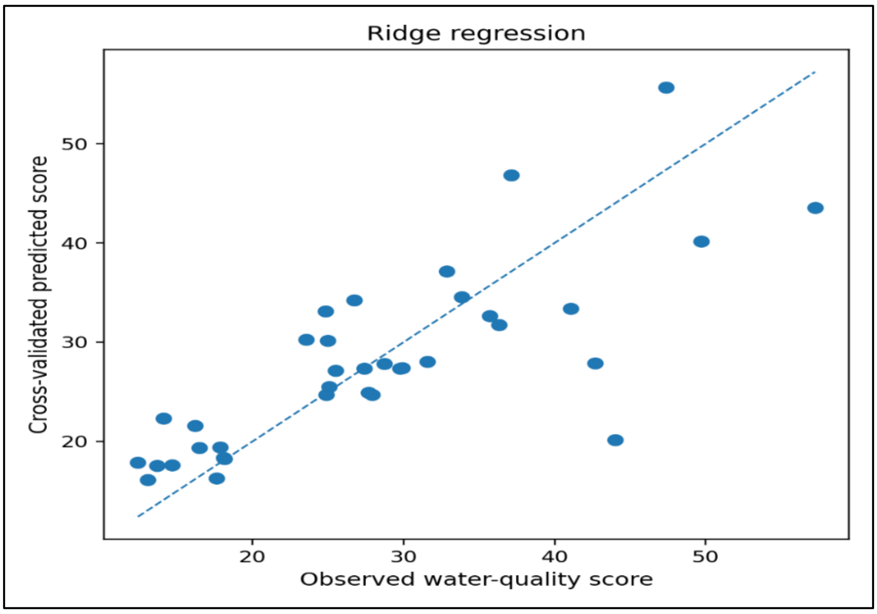


**Figure 3. Observed Versus Cross-Validated Predicted Water-Quality Scores Using Ridge Regression**

## 4. Discussion

Results indicate significant differences in water-quality between the three monitoring sites, with moderate differences between seasons. The highest value of integrated water-quality score and COD was obtained from Jabalpur and the lowest value was obtained from Anuppur. High turbidity, dissolved oxygen and rainfall were some of the characteristics of Dindori. This spatial heterogeneity is entirely in line with evidence of spatial variability in water chemistry in the same freshwater system due to variations in catchment characteristics, pollutant inputs and local environmental processes. Comparable spatial and temporal separation were found in Lake Hawassa where a multivariate evaluation found water-quality patterns and possible pollution sources in the monitoring areas (Lencha et al., 2021). The presence of spatial variability in the physicochemical parameters of Jhelum River has also been shown and assessing the water quality indices (WQI) is location-specific (Ahmad et al., 2024).

Strong positive relationships with the integrated score for the total coliform, phosphate, BOD, conductivity, dissolved solids, and COD data suggest that water-quality impairment was a result of a combination of stressors and not a single dominant parameter. BOD and COD indicates organic and oxidizable loads and conductivity and dissolved solids indicates dissolved ionic material. Physicochemical measurements are still critical to integrated water-quality assessment because using a combination of various measurements can yield better picture of the water pollution status than a single parameter measurement (Nayar, 2020). River pollution indicators also show the benefit of considering both chemical and physical factors for looking at river water quality (Alwan & Saeed, 2024).

Environmental factors were more intricate. The relationship with the integrated outcome was positive with water level but not significant with rainfall. The lack of a good direct rainfall relationship does not mean that hydrological conditions are of no consideration as rainfall affects water through runoff, dilution, transport and delayed catchment responses. Studies of water systems in rural Africa show that precipitation displays significant intra-seasonal fluctuations and can have a significant impact on water-related processes on relatively short time scales (Armstrong et al., 2022). This observed seasonal overlap might thus be a result of an interaction between hydrological conditions and local physicochemical conditions and not necessarily a consistent seasonal response.

Water quality was also estimated using machine-learning analysis yielding further evidence that water quality could be estimated from available predictors. Ridge Regression had the best overall cross-validated performance ($R^2 = 0.603$) with Random Forest just behind ($R^2 = 0.575$). The regularized linear model indicates that a significant part of the predictive structure might be captured without being too complicated for the algorithm. Machine learning has become a more and more valuable analytical tool, connecting multidimensional observations and recognizing relationships that are not easily discerned from traditional methods, and thereby increasingly contributing to environmental science (Zhong et al., 2021). The importance of predictive methods for converting environmental measurements to actionable information about water quality is also evident in remote sensing and machine-learning research in the field of lake management (Deng et al., 2024).

The higher structural flexibility of Decision Tree Regression also suggests that bigness doesn't necessarily imply goodness, when the number of observations is not that large. A similar study of environmental modelling has revealed that the choice of model should be guided by the spatial and temporal structure of the environmental process, which is not only dependent on the complexity of the algorithm (Ren et al., 2020). In addition, in ecological applications, machine learning is only informative if the predictive performance is complemented with an interpretable ecological insight (Yu et al., 2021). This consideration is particularly pertinent in the present context because the main importance of prediction is not just to estimate the water-quality scores, but to know how the environmental and physicochemical conditions influence the water-quality scores. Interpretable predictive modelling is useful in general, as machine learning algorithms are increasingly being used to aid variable selection and pattern discovery in large and complex biological datasets (Elguoshy et al., 2025).

Applied, incorporation of routine water measurements with environmental information may help to enhance monitoring and prioritisation of key indicators that have influence. However there are some caveats to be noted. The number of observations in the dataset was only 36, which is low compared to the complexity of the model and generalizability, and the integrated outcome was based on the indicators available in the data. These relationships should be confirmed in the future using larger data sets with several years of data and extended monitoring networks and climatic and catchment data.

## 5. Conclusion

This study indicates the usefulness of combining the physicochemical, environmental, spatial and hydrological indicators for the data-driven water-quality assessment. The spatial variations were quite prominent at Anuppur, Dindori and Jabalpur but seasonal differences were relatively small. Jabalpur was found to have the best mean integrated water-quality score while Anuppur had the lowest score. The parameters of total coliform, phosphate, BOD, conductivity, dissolved solids, and COD showed strong relationships to increasing water-quality impairment, suggesting that microbial contamination, nutrient enrichment, organic loading and dissolved ionic constituents all contributed to water-quality impairment. Analysis of machine-learning using cross-validated predictive performance showed the best results for Ridge Regression ($R^2 = 0.603$; RMSE = 6.98) and comparable results with the lowest MAE for Random Forest. The results suggest that a relatively simple model can be developed that will provide useful predictive information from the multidimensional water-quality measurements without being overly complicated. The framework has real potential for prioritising indicators that are influential, and enabling targeted environmental monitoring. The sample however, is quite small (36 observations) and this does not allow for any wider generalization. Future validation with larger, multi-year monitoring data would help to increase the confidence in prediction and to extrapolate to operational water-resource management.

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