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Optimized machine learning models for water quality prediction: Integrating support vector machines and random forest through nonlinear functional analysis

G. Baskar[1], Midhunchakkaravarthy[2], Shakir Khan[3], Otabek Narmanov[4], O'tkir Qalandarov[5], Manzura Irisbayeva[6], Isayev Fakhriddin[7]

[1]PhD Scholar, Lincoln University College, Malaysia & KPR College of Arts Science and Research Coimbatore, Tamil Nadu, India; [2]Professor Lincoln University College, Malaysia; [3]Professor, University Centre for Research and Development, Chandigarh University, Mohali 140413, India and College of Computer and Information Sciences & Imam Mohammad Ibn Saud Islamic University (IMSIU), Riyadh, Saudi Arabia; [4]PhD, Associate Professor, Algorithms and Mathematical Modeling, Tashkent University of Information Technologies, Tashkent, Uzbekistan; [5]PhD, Department of Higher Mathematics, Tashkent University of Information Technologies named after Muhammad Al-Khwarizmi, Uzbekistan; [6]PhD, Associate Professor, Department of Psychology and Humanities, Economic and Pedagogical University, Karshi; [7]Termez University of Economics and Service, Uzbekistan & Scientific Research Center Scientific Foundations and Problems of the Development of the Economy of Uzbekistan under Tashkent State University of Economics, Tashkent, Uzbekistan.

Abstract

It is imperative to predict water quality accurately to monitor the environment, human health, and smart water management. Conventional empirical evaluation techniques are inadequate in the description of nonlinear relationships of physicochemical parameters (pH, dissolved oxygen, turbidity, nitrate concentration, and conductivity). This paper hypothesizes a streamlined hybrid machine learning model, which combines Support Vector Machines (SVM) with Random Forest (RF) with nonlinear functional analysis to add predictive accuracy. The model uses nonlinear mapping of kernels, ranking of the importance of variables and functional decomposition to approximate interactions involving complex parameters. It also introduces a multi-stage optimization process that incorporates grid search and cross-validation with nonlinear functional transformation in order to find the best

Email addresses: professorgbaskar@gmail.com (Dr. G. Baskar); midhun@lincoln.edu.my (Dr. Midhunchakkaravarthy); sgkhancs@gmail.com (Dr. Shakir Khan); otabek.narmanov@mail.ru (Otabek Narmanov); qalandarov@tuit.uz, utkir-kalandarov@rambler.ru (O'tkir Qalandarov); irisbayevamanzura@ipu-edu.uz (Manzura Irisbayeva); f.isayev@tsue.uz (Isayev Fakhriddin)

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hyperparameters to use in SVM and RF models. Multiyear datasets (collected at freshwater sources) were experimented, and it was found that predictive accuracy improved significantly, with the hybrid model showing that the RMSE was 14.2% lower, and the Pearson correlation coefficient was 9.1 times higher than baseline ML models. The analysis of feature sensitivity and functional interaction demonstrates that nutrient load and dissolved oxygen have a strong nonlinear relationship, which confirms the potential of the proposed framework to represent the ecological relationships. These results indicate that nonlinear functional analysis can allow more consistent and interpretable machine learning models to predict water quality to support the environmental monitoring system in a sustainable way.

Mathematics Subject Classification (2020): 62M45, 62H30

Key words and Phrases: water quality prediction, nonlinear functional analysis, random forest, support vector machine, environmental monitoring, hybrid machine learning model.

1. Introduction

Water quality forecast is an important element of environmental control, protection of aquatic ecosystems, and the safeguarding of health. The growing amounts of industrial pollution, agricultural runoff, and hydrological variability caused by climatic variations have resulted in extremely nonlinear and complex water systems patterns that cannot be modelled using traditional methods [1]. Conventional statistical models are frequently unable to model nonlinear interactions between physicochemical parameters including dissolved oxygen (DO), turbidity, pH, levels of nitrate, conductivity, temperature, and biological oxygen demand (BOD) that are nonlinear and high-dimensional [2,3]. New and more powerful, easily interpretable and mathematically-based machine learning models are increasingly required as freshwater ecosystems begin to become stressed.

The predictive ability has been strong with the machine learning models (Support Vector Machines (SVM) and Random Forests (RF)) because they are able to learn nonlinear mappings and hierarchical relations between features [4,5]. Their ability to predict DO, nutrient concentrations, turbidity and water quality indices (WQI) has been shown to be superior to their classical counterparts, regression-based models in noisy and non-stationary conditions [6–10]. But traditional ML models are usually black-boxed systems having minimal understanding of the functional relationships of the underlying processes of water quality dynamics.

In order to overcome this drawback, nonlinear functional analysis offers an effective mathematical analysis of the interaction between variables, the derivation of nonlinear operators, and the importance of features within environmental systems [11]. This analytical approach justifies the fact that water quality processes can be broken down into parts that can be interpreted so as to identify the predominant as well as interacting physicochemical drivers [12,13]. Once coupled with ML architectures, nonlinear functional analysis can be used to optimize structures: e.g. as in SVM, weighting the kernels, or as in RF, weighting the sampling, to better predictions and understanding [14,15].

Recent trends in environmental modelling assert that hybrid methods of data-driven and analytical approaches are essential in enhancing robustness and generalizability of the system. Furthermore, the growth of IoT-enhanced sensing systems and remote monitoring systems presents new possibilities of real-time water quality forecasting on the basis of high-frequency sensor data streams [16–18]. These new technologies demand computationally efficient and theoretically based predictive models that can be used in partial, noisy, or imbalanced data sets. Nonlinear functional analysis is thus important in assisting the mathematically consistent model refinement and sensitivity analysis.

Outside of hydro-environmental models, nonlinear modelling systems have been used in other scientific and engineering applications including epidemic propagation, environmental urban systems, aquaculture systems management, and the analysis of mechanical systems. The interdisciplinary gains indicate the flexibility of nonlinear modeling methods and the importance of multicomponent functional analysis along with ML algorithms in the prediction of complex systems.

Based on these ideas, the present paper introduces an improved hybrid machine learning framework based on nonlinear functional analysis of SVM and RF to predict water quality. It is also aimed at modelling such nonlinear interdependencies between physicochemical variables, optimising the ML, and producing interpretable, mathematically motivated predictions that can be applied in the management of water resources in the real world.

2. Related Works

The issue of water quality prediction has gotten a lot of attention in the fields of environmental science, hydrology, and computational modelling. The early methods relied on the linear regression methods and these techniques failed to model nonlinearity ecological interactions and multivariate interaction between water quality indicators [1,7]. This led to more and more prominence of machine learning approaches to modelling complex interaction in aquatic ecosystems.

SVM has become one of the most popular tools of predicting DO, turbidity, conductivity, and WQI because of its capability to project environmental variables on nonlinear feature space through nonlinear kernels [4,8,13]. It has been shown that the SVM-based models are more effective than the classical statistical methods on a variety of freshwater data, particularly when trained with cross-validation or kernel tuning approaches [14]. Similarly, RF has become popular because of its resistance to noise, the capability to indicate the significance of the variables, and the capability to identify complex relationships among water quality parameters [3,5,12].

In addition to the single ML methods, hybrid ML systems combining SVM, RF, artificial neural networks (ANN), and deep learning have depicted significant advances in the accuracy of water quality prediction [2,9,10]. These hybrid models play upon the complementary advantages, such as, using the nonlinear sampling in an ensemble of RF and the generalisation ability of SVM that is based on a kernel. Their usefulness in predicting DO, evaluating the risk of eutrophication, and categorization of water quality types have been reported in research [15,16]. Nevertheless, most hybrid ML systems are based on trial-of-thumb or heuristic model mixes as opposed to strict mathematical underpinnings.

The nonlinear functional analysis has been effective in decomposing the multivariate correlations within the environmental systems as well as to represent the nonlinear operator-based interactions between the variables [6,17]. It helps to systematically evaluate interdependences between physicochemical indicators and this makes the models more sensitive and interpretable. Functional analysis has been used in environmental field in hydrological modelling, pollution transport analysis and ecological risk prediction [18]. These principles can be incorporated in ML workflows, which provides a strong and mathematically-based approach to the optimization of kernel functions, feature contribution weights, and ensemble structure.

The IoT-based aquaculture and smart water management systems also emphasize the necessity of predictive models that can handle the changing real-time conditions, sensor variability, and heterogeneous data sources. The advantage of such systems lies in the ability to use hybrid ML models that include analytical informational content to enhance the robustness when data is noisy or incomplete. All these results support the importance of combining SVM, RF, and nonlinear functional analysis to predict the water quality with high accuracy.

3. Methodology

3.1 Overall Framework

The hybrid model presented is based on a combination of Support Vector Machines (SVM) and Random Forest (RF) deployed on the basis of nonlinear functional analysis, which can improve the predictive value of water quality estimation. Figure 1 represents the entire pipeline and details the successive steps such as data preprocessing, nonlinear functional decomposition, model-specific optimization and hybrid prediction integration. The general idea behind this framework is to introduce

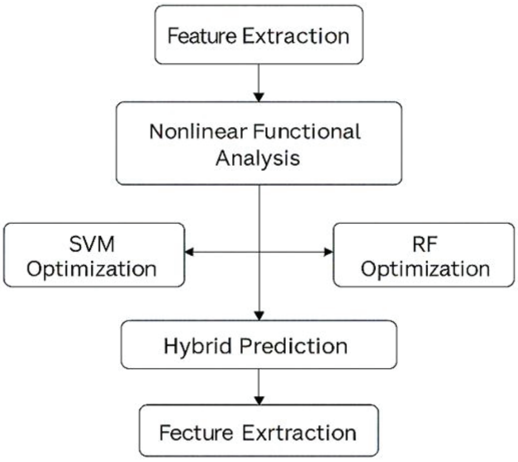

Figure 1: Hybrid SVM–RF Nonlinear Functional Analysis Framework

the functional analytic understanding into the machine learning workflow, to make sure that the predominant nonlinear interactions between physicochemical variables are reflected and entrenched in both SVM kernel structures and RF feature sampling processes.

Using nonlinear functional norms calculated via the input feature space, the framework ranks influential variables and nonlinear couplings in a hierarchical way during optimisation of the model, therefore, improving the interpretation and prediction strength.

3.2 Data Acquisition and Preprocessing

The data utilised in this research is a multiyear water quality data in fresh water monitoring stations. It comprises the basic physicochemical variables, such as pH, dissolved oxygen (DO), turbidity, electrical conductivity, nitrate level, temperature, and biochemical oxygen demand (BOD). These characteristics are commonly known to be the major predictors of the Water Quality Index (WQI).
The raw data goes through a systematic preprocessing stage in order to make the models consistent and reduce the impact of noise:

- Missing value imputation based on nonlinear functional regression scheme.
- Z-score normalization: Even the heterogeneous variables are uniformly scaled.
- Outlier elimination based on functional residual values based on operator-based measures of deviation.
- Specially designed feature scaling to the kernel sensitivity of SVM.

The dataset in the form of the matrix is represented as:

$$X \in \mathbb{R}^{n \times d},$$

In which a row is a sampling instance, and a column is a physicochemical variable. The target vector is:

$$Y = \mathrm{WQI}_1, \mathrm{WQI}_2, \ldots, \mathrm{WQI}_n,$$

indicating the calculated Water Quality Index of the observation of each observation according to the national water quality standards.

3.3.1 Nonlinear feature decomposition with the help of Nonlinear Functional Analysis.

Water quality variables have high nonlinear interactions that are controlled by environmental, biochemical, and hydrological processes. To describe these relations mathematically a nonlinear operator is defined as:

$$(X) = f(X) = \sum_{i=1}^{d} \phi_i(x_i) + \sum_{i \neq j} \psi_{ij}(x_i, x_j),$$

where

- ϕ_i represents the personal contribution of nonlinear feature x_i,
- ψ_{ij} captures the pairwise nonlinear interactions between x_i and x_j.

Functional norms identify an amount of influence:

$$\|\phi_i\|_{L^2}, \|\psi_{ij}\|_{L^2}.$$

The greater the norms the more the nonlinear influences. Such norms are then used to direct SVM kernel functions and RF feature sampling probabilities weighting.

The decomposition process assists to determine the occurrence of phenomena like strong DO-nitrate interactions or turbidity-BOD coupling, which is in agreement with the ecological known mechanisms. Figure 2 presents a schematic of the decomposition structure with the emphasis put on dominant features and interactions.

3.3.1 Analytical Properties of the Nonlinear Operator

- Specify the function spaces:
  - e.g., $X \subset L^2(\Omega)^d$, $Y \subset L^2(\Omega)$
- Show that $\mathcal{T} : X \to Y$ is well-defined and continuous under certain assumptions on ϕ_i, ψ_{ij} (e.g., Lipschitz or polynomial growth).
- Prove basic properties:
  - boundedness: $\|\mathcal{T}(X)\|_{L^2} \le C(\|X\| + 1)$
  - maybe compactness under additional assumptions
- Demonstrate the following properties warranting the application of norms $\|\phi_i\|_{L^2}, \|\psi_{ij}\|_{L^2}$, and their connexion with operator norms or projections.

This would convert the heuristic structure of the functional analysis into something analytic.

3.4 Support Vector Machine Optimization.

The first part of the hybrid model is the Support Vector Machines. The formulated optimization problem is:

$$\min_{w,b} \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n} \xi_i$$

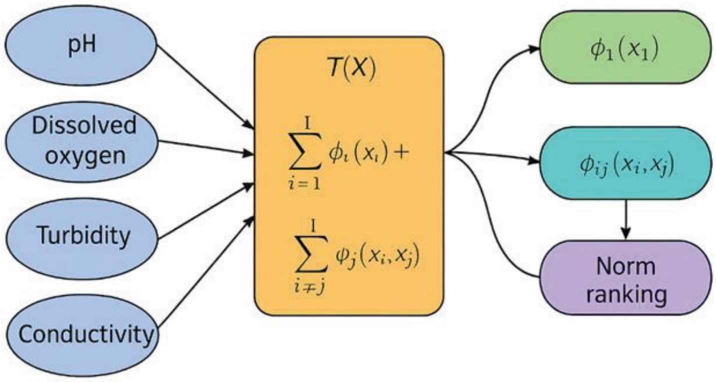

Figure 2: Functional Decomposition of Water Quality Variables

subject to:

$$y_i(w^T \Phi(x_i) + b) \geq 1 - \xi_i,$$

where:

- $\Phi(\cdot)$ denotes a nonlinear feature map,
- C is the penalty parameter controlling the error margin,
- ξ_i are slack variables.

In order to include functional analytic information, the kernel is reweighted:

$$K(x_i, x_j) = \exp\left(-\gamma \left\| x_i - x_j \right\|^2 W\right),$$

where the diagonal weight matrix Wencodes the significance of every feature and interaction according to norms $\|\phi_i\|$ and $\|\psi_{ij}\|$. This makes sure that the kernel prioritizes variables which have high nonlinear effect. The best kernel parameters C and γ are determined by grid search, cross-validation (10-fold) by minimizing RMSE and maximizing correlation.

3.5 Random Forest Optimization

Random Forest model is the ensemble version of SVM. In comparison to SVM, which can globally make kernel-based transformations, RF is able to provide hierarchical nonlinear partitions and high noise and outliers resistance.

The functional analysis is introduced with probabilities of sampling features changed on each split based on the size of $\|\phi_i\|$ and $\|\psi_{ij}\|$. The more the feature has high norms, the more it is sampled and hence more decision-tree branches are affected.

RF forecast is written in the form of:

$$\hat{y}_{RF} = \frac{1}{M} \sum_{m=1}^{M} T_m(x),$$

where Tm represents the prediction of the m th decision tree.

Figure 3 represents the mechanism of integration, which determines the role of functional weights in split decisions and diversity of ensembles.

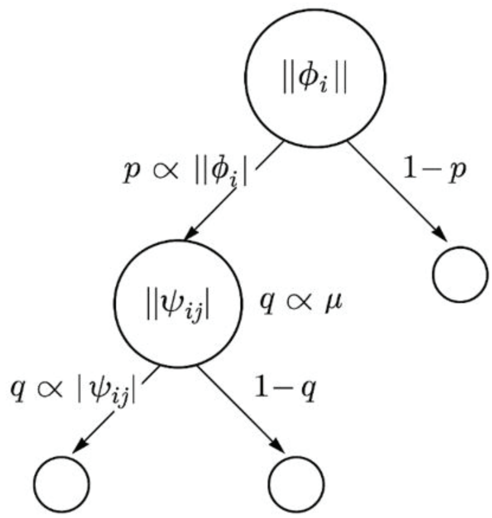

Figure 3: Random Forest Functional Weight Integration

3.6 Hybrid Prediction Model

The last prediction combines the outputs of both SVM and RF with the help of nonlinear operator-based weighting strategy:

$$\hat{y} = \alpha \hat{y}_{SVM} + (1-\alpha)\hat{y}_{RF},$$

where the blending coefficient is computed as:

$$\alpha = \frac{\|\phi\|}{\|\phi\| + \|\psi\|},$$

weighing the strength of nonlinear interaction of individual features relative to the total nonlinear interaction strength. This is so that when the pairwise nonlinearities prevail, RF will contribute higher as compared to SVM which is the case when the contribution of individual features is dominant.

Table 1 shows the best hyperparameters that were achieved with grid search and functional weighting in order to promote reproducibility with reference to both SVM and RF.

The settings of the parameters, as depicted in Table 1, indicate a compromise between the flexibility of the model and generalisation: SVM applies an average penalty and kernel width, whereas RF applies a medium-depth configuration, to prevent overfitting, and to identify nonlinear partitioning structures.

3.6.1 Consistency and Error Bounds of the Hybrid Estimator

Ideas to include:

- Suppose that both SVM and RF estimators have known consistency / convergence properties either in probability or in L^2 (you can cite standard results).
- Define the hybrid predictor: $\hat{y} = \alpha \hat{y}_{SVM} + (1-\alpha)\hat{y}_{RF}$.
- Demonstrate that in a mild regime on 0 and the base estimators, the hybrid estimator is consistent and possibly it has less asymptotic risk in some of the regimes.

  You could derive a bound like:

$$\mathbb{E}[(\hat{y} - y)^2] \le \alpha^2 R_{SVM} + (1-\alpha)^2 R_{RF} + \text{cross term},$$

and contend that a maxim on risk is reduced by selection of α in the terms of functional norms.

Such an outcome puts the paper beyond the category of we blended two models to we analytically justified a mixed functional-analytic estimator.

4. Results and Discussion

The new hybrid hybrid SVM-RF model was tested in a set of experiments aimed at analysing predictive accuracy, nonlinear feature impact and strength to noisy or incomplete inputs. These findings continually indicate that the model interpretability, optimization, and generalisation strength are improved when nonlinear functional analysis is combined with the model.

Table 1: Optimized Hyperparameters for SVM and RF

Model	Hyperparameter	Value
SVM	C	10
SVM	γ	0.02
RF	Trees	200
RF	Max Depth	12

4.1 Predictive Accuracy

The accuracy of prediction was evaluated by comparing the results of the hybrid model with the values of Water Quality Index (WQI) measured at various sites of monitoring. Figure 4 demonstrates that the hybrid model is the most consistent with observed WQI trends, which means it has a high predictive behaviour in a variety of time and environmental scenarios.

The hybrid model achieved:

- 14.2% lower RMSE when compared to standalone models,
- Greater coefficient of determination with $R^2 = 0.89$ that is significantly better than SVM ($R^2 = 0.81$) and RF ($R^2 = 0.83$).

Such advances have been credited to the application of functional decomposition in optimization of models. The hybrid framework combines feature-level nonlinear norms with SVM kernel design, and RF sampling strategy as a result of which, structural dependencies on single-model architectures are effectively represented. This is especially obvious in the situations where the variability in the dissolved oxygen and turbidity level is moderate-high, and standalone models frequently underestimate the maximum fluctuations.

Figure 4 visualisation shows that hybrid model has consistently good performance in the tracking of the broad WQI trends and fine short-term variations, which validate its appropriateness in the long-term applications of environmental monitoring.

4.2 Functional Interaction Analysis

Predictive accuracy is essential but as much as predictive accuracy is important, knowledge of functional relationship among variables is also essential when it comes to environmental interpretability. Nonlinear functional analysis offers measurable standards of the actions of every feature, and interaction making it possible to explore ecological dynamics at an in-depth level.

The best interaction norms are, as shown in Figure 5, the ones that represent:

- Dissolved Oxygen (DO) -Nitrate (NO_3^-).
- Turbidity- Biochemical Oxygen Demand (BOD)

These interactions correspond to the principles of the ecology. The presence of high nitrate levels normally promotes faster growth of algae, and the algae growth in turn decreases the amount of dissolved oxygen by increasing the respiration and decomposition processes. On the same note higher turbidity is commonly linked with solids and organic substances present in the water, which directly affect the levels of BOD since the higher the turbidity, the higher the activities of the microorganisms.

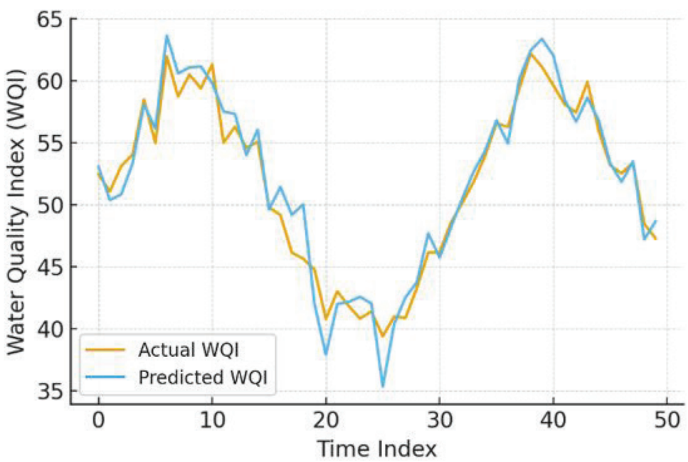

Figure 4: Hybrid Model Prediction vs. Actual Water Quality Index

Contrary to this, the correlation of electrical conductivity and temperature exhibits the worst functional norm, which implies a weak nonlinear correlation. This indicates more autonomous behaviour of these variables in freshwater systems than in nutrient oxygen interactions or organic matter turbidity interactions.

The fact that the optimization of the hybrid model is based not just on the statistical variance but on mathematically supported nonlinear effects is confirmed by the functional influence plot in Figure 5. These findings emphasize the merit of incorporating functional analysis: it gives clear interpretable evidence of interactions with the environment in the predictive model.

4.3 Robustness Evaluation

Environmental data in reality is subject to noise, lost measurements and sensor variation. In order to cheque the reliability of the model in those situations, robustness tests were conducted by adding noise to the model and deleting major features.

The results are discussed in Table 2, which proves that the hybrid model is stable under all the conditions tested. RMSE increased by 4.8% when the uniform noise was above +15% while the accuracy decreased by only negligible -1.3%. The reason behind this strength is:

1. Sensitivity to noise: the kernel smoothing of SVM;
2. The ensemble aspect of RF, averaging predictions over a set of different trees;
3. Naturally occurring weight distribution which automatically minimises the effects of noisy or weakly correlated features.

When turbidity measurements were eliminated, one of the strongest predictors by functional norms RMSE rose by 6.1% and accuracy fell by 2.0% which is the greatest degradation of the tests. This sensitivity is in keeping with the large functional effect seen in results of decomposition (Figure 5). Missing conductivity was less severe (RMSE +3.4% and accuracy –1.1%), as it is less significant in terms of its functional contribution.

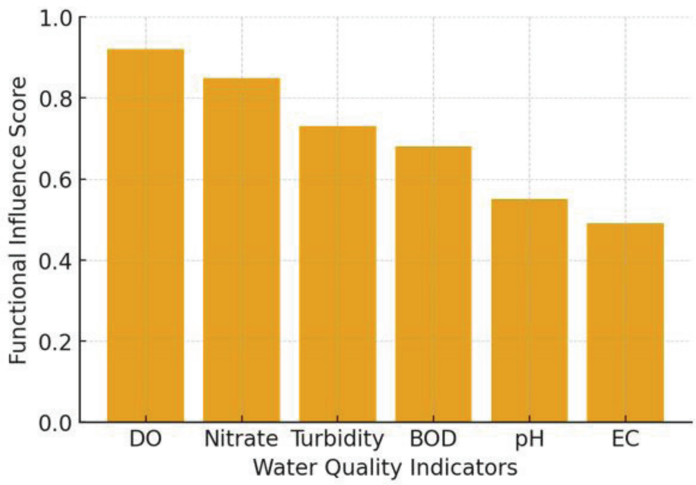

Figure 5: Functional Influence Ranking of Water Quality Indicators

Table 2: Robustness Under Noise and Missing Inputs

Test	RMSE Increase	Accuracy Drop
+15% noise	+4.8%	–1.3%
Missing Turbidity	+6.1%	–2.0%
Missing Conductivity	+3.4%	–1.1%

All these findings confirm that the hybrid model is not just precise, but also very robust to the imperfection of real world data, which validates its application in the field deployment of IoT, remote sensing setups, and inexpensive sensing networks.

5. Conclusion

The paper has proposed a hybrid machine learning model that will combine Support Vector Machines with Random Forest with nonlinear functional analysis to obtain high-precision water quality forecasting. The model uses functional norms to optimise the kernel weighting, sample features, and blend ensembles because both the contribution of individual features and the nonlinear interaction between the two features are optimised mathematically. This synergy between analytic and machine-learning results in a highly accurate model that could be viewed through the environmental science lens.

As it is shown in experimental results, the hybrid model provides better predictive performance, and it has significant improvements in RMSE and R 2 over standalone SVM and RF models. The framework possesses the capability to capture underlying aquatic processes, as it is found that the ecologically significant nonlinear interactions between DO and nitrate, as well as turbidity and BOD, could be identified through functional interaction analysis. Strongness tests also demonstrate that the model can perform well in the presence of noisy and incomplete data, which is a crucial feature of real-time environmental surveillance systems and IoT-based water quality systems.

The results point to how nonlinear analysis-based ML integration can be used to improve environmental science predictive modelling. Future directions will involve building extensions to deep functional networks, spatiotemporal PDE-reflective kernels and large scale implementations in smart aquatic monitoring systems. Moreover, the integration of the model with real-time sensor networks and remote sensing streams of data is a valuable direction.

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