# Seasonal Spatio-Temporal Machine Learning with Conformal Uncertainty for Forecasting Nitrate, Ammonia, and Orthophosphate in Surface Waters

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**Citation |** Tehseen. R, Mustaqeem. A, Haq. M. I. U, Awan. M. M, Omer. U, Inayat. W, Rafaqat. S, "Seasonal Spatio-Temporal Machine Learning with Conformal Uncertainty for Forecasting Nitrate, Ammonia, and Orthophosphate in Surface Waters", IJIST, Vol. 08 Issue. 01 pp 179-195, January 2026
**Received |** December 16, 2025 **Revised |** January 12, 2026 **Accepted |** January 17, 2026 **Published |** January 22, 2026.

Proper prediction of nutrient contents in organizations is critical to safeguarding water bodies as well as sustainable environmental management. This article introduces a seasonal spatio-temporal prediction framework of nutrients based on machine learning and estimation of uncertainty. Based on the large-scale monitoring data in 2010-2025, monthly concentrations of nitrate, ammonia, and orthophosphate were modeled at thousands of sampling sites. Fast features: Feature engineering. The temporal dynamics were modeled using seasonal encoding, lag values, and rolling statistics. Three prediction methods were considered: the Random Forest regression, the XGBoost regression, the feed-forward neural networks, and the hybrid model that concluded with the combination of the Random Forest and the neural network learning. Conformal prediction was used to measure prediction uncertainty to produce statistically sound 90 percent prediction intervals. Mean absolute error, root mean square error, coefficient of determination, and interval coverage were used to determine model performance. It was found that the overall performance of Random Forest with conformal prediction (MAE = 0.1008, RMSE = 0.2294, R2 = 0.7746) is the best, followed by the hybrid residual model, presenting the reported results are averaged across nutrients. XGBoost and neural network models also showed a high predictive power, but the accuracy of the models and the uncertainty confidence limits were lower. Significantly lower performance was exhibited by baseline persistence and climatology methods. ANOVA was required to test whether the performance difference of the models was due to statistically significant variation. The solution offered by the suggested framework is accurate, interpretable, and error-aware in the long-term nutrient forecasting. The methodology provides credible data concerning environmental risks and sound decisions on water quality management through the combination of ensemble learning and conformal uncertainty estimation.

**Keywords:** Water Quality, XGBoost, Random Forest, Forecasting, Anova

**Introduction:**

Maintenance of human health, ecological level, agricultural output, and economy. Surface water resources like rivers, lakes, and reservoirs are the main sources of drinking water, irrigation, industrial use, and aquatic systems. Of many parameters that are commonly used to assess the quality of water, nutrient levels, especially nitrate, ammonia, and orthophosphate, are considered to be important parameters due to their high impact on water eutrophication, algal proliferation, reduction of oxygen, and eventual destruction of the ecosystems [1][2][3][4]. The overloading of nutrients does not just alter the aquatic biodiversity, but also raises costs of treatment, as well as having health hazards when water contaminated by the excess is consumed in the household and its use by farmers [5][6][7]. Surface waters are very complex with respect to nutrient dynamics. These concentrations are different in space depending on the land-use, agricultural runoff, urban discharge, and hydrological connectivity. Simultaneously, the nutrient content varies with time owing to the rainfall in the season, temperatures, life activities, and man-made actions. Such spatio-temporal fluctuations do not ensure an easy prediction of nutrients, especially in cases when the data are scattered, discontinuous, or unbalanced both spatially and in time [8][9][10]. Such nonlinear and interacting processes can be difficult to model using traditional statistical models and restrict the extent to which they can be predictive in reality [11][12]. The latest developments in machine learning and deep learning have brought in strong substitutes to model complex environmental systems. Random forests, gradient boosting, artificial neural networks, and recurrent neural networks are algorithms that have a high potential for predicting water quality in various geographic locations and chemical parameters [1][13][14][15][16]. These models can learn nonlinearly, without knowledge of explicit physical equations, making them appropriate for heterogeneous datasets of the environment. A variety of research studies have effectively used machine learning to forecast groundwater nitrate, arsenic, manganese, PFAS, and other contaminants more accurately than the traditional methods [17][18][19][7][20]. Although these developments have taken place, there are a number of significant constraints. To begin with, a number of current research studies have all been largely centered on groundwater instead of surface water systems despite the fact that the former is more susceptible to seasonal climatic fluctuation and human activity [2][3]. Second, most of the prediction models focus on one of the contaminants, whereas management of water quality in reality needs a combination of knowledge on a combination of interacting nutrients like nitrate, ammonia, and orthophosphate [21]. Third, in spite of the fact that temporal forecasting is referenced, it is a relatively new field with only a few applications taking into account the real variegated factors, locational particular and momentary [22] in the genuine representativeness of spatial-temporal modeling. The other serious challenge is uncertainty.

The predictions given by machine learning models are usually point predictions, and they will have no information as to confidence or reliability. Uncertainty information is needed in environmental decision-making. Policy makers, community, and water managers should not only be aware of the forecasted nutrient concentration, but also be aware of the upper and lower limits within which the actual value could fall. The lack of quantification of uncertainty also means that even very accurate predictions can give dangerous or risky decisions [4][6]. More recent studies have shown the significance of uncertainty-aware modeling using probabilistic learning, ensemble methods, Bayesian, and conformal prediction techniques, but these methods have not been explored significantly in nutrient prediction research, and more so with surface waters [23]. Nutrient behavior is also made difficult by seasonality. The movement and changes in nutrients are highly dependent on the seasonal rainfall, temperatures, agricultural seasons, and biological activities. The application of models based on neglect of seasonal behavior may yield poor performance and may become difficult to interpret. and several studies have provided evidence that the inclusion of the seasonal or

periodic element enhances predictive activity in hydrological and water quality forecasting. Implicitly, however, seasonal modeling is used without explicit consideration to be implemented in spatiotemporal machine learning systems. On a practical note, predictability in nutrient awareness is directly of value to society and economics. The water treatment facilities depend on early notifications in order to change the purification processes. Water quality in agricultural planning would prevent crop losses due to the destruction of the crop. Societies need available resources to evaluate the safety of surface water for either domestic or recreational use. Having nutrient levels that are above the regulatory levels, water can become inappropriate to consume, irrigate, or sustain an ecosystem, thereby enhancing water scarcity, although the amount of water is physically available. Thus, NG prediction systems with proper accuracy and uncertainty knowledge can be utilized to lead to such cost-effective water management and risk-based decision making. Despite tremendous studies on the prediction of water quality, there is a dearth of an integrated framework that comes up with multiple nutrients, at the same time, spatiotemporal variability, seasonal cycle, and predictive uncertainty of surface water systems. Most of the available works are based on either a pure time and spatial approach or a spatial approach alone; however, the physical environmental systems work in both aspects simultaneously.

Moreover, the literature concerning the comparative assessment of machine learning, deep learning, and hybrid modeling approaches in the context of a single uncertain aware approach is limited. To overcome these shortcomings, models needed in forecasting the nutrient concentration must be able to: (1) measure nonlinear interactions between the environmental features and nutrient dynamics, (2) are explicit representations of seasonal periodicity, (3) consider spatial and time heterogeneity between locations of monitoring, (4) give meaningful and valid uncertainty estimates as well as point predictions, and (5) facilitate the practice interpretation in the assessment and management of water quality. This type of framework is capable of providing early warning of events of nutrient excess, assisting regulatory compliance, and even decreasing the cost of treatment and monitoring over time. More to the point, it may be used to translate crude environmental information into knowledge applicable to preserving human health and aquatic organisms. It is against this light that the world seasonal spatiotemporal nutrient prediction model with a consciousness of the level of uncertainty is a requisite consideration towards increasingly plausible and decision-making orientated surface water quality modeling. Demonstrating an emphasis in the analysis of nutrient dynamics focusing on nitrate, ammonia, and orthophosphate, machine learning, deep learning, and the combination of machine learning and conformal uncertainty estimates may provide better accuracy, trustworthiness, and practical significance to the discussion. The obtained predictions have a chance to be used by water authorities, researchers, and local communities to analyze the usability of water in the future and recognize the threats of contamination of water before it is too late to take appropriate measures.

**Literature Review:**

The situation with the deterioration of water quality has become a worldwide environmental issue because of the quick development of the industry, intensive farming, urbanization, and climate change. Such nutrients as nitrate, ammonia, and orthophosphate are among other contaminants that dominate in damaging the aquatic environments and endangering the drinking water safety. The sources of these nutrients are mainly as a result of fertilizer runoff, animal waste, sewage outflow, and atmospheric deposition, which consequently result in the extensive eutrophication, oxygen depletion, and ecological imbalances in the surface and underground water systems. High levels of nitrate have been linked to severe effects on human health, such as methemoglobinemia and possible carcinogenic conditions, and ammonia and orthophosphate play a major role in algal outbursts and biodiversity loss. Strict limits on threshold concentrations of nutrients in drinking and

environmental water are thus enforced in all parts of the world by regulatory organizations. Nonetheless, the constant testing of the nutrient levels is costly, logistically not ideal, and in some instances, it is spatially limited, particularly in that of the developing world. Such constraints have promoted the establishment of forecast models that can predict future nutrition behavior based on environmental information available.

The initial predictive methods of water quality were relatively dependent on statistical regression, correlation, and the detection of trends. The growth of water quality trends over the long term and the effects of climatic factors were commonly conducted through seasonal decomposition and linear regression models. These approaches were very interpretable, but failed to describe nonlinear interactions among the nutrient concentrations with the determinants of land use, hydrology, and climate variability. As a result, the accuracy of prediction could still not be reached in complex natural systems. The implementation of machine learning also had a tremendous contribution to the water quality modeling through the ability to recognize nonlinear patterns using large volumes of data. The decision trees, support vector machine, the random forest, and the gradient boosting models had better results than the conventional statistical methods in predicting ground water contaminants and surface water contaminants. Machine learning models in groundwater research were able to forecast the concentration of nitrates with geographic, climatic, and land use variables even in areas with little data. Random forest and gradient boosting appeared to be highly robust and generalized well as ensemble models].

There is also the multi-contaminant modeling. Multilabel and semi-supervised learning approaches to machine learning have been utilized to predict several PFAS compounds concurrently. The same has been employed to estimate the amount of arsenic and manganese in aquifer systems and has shown a high spatial heterogeneity in the arsenic and manganese contamination patterns. These experiments proved that machine learning offers an effective instrument to rely upon when assessing water quality at its region and nation level. Machine learning has been used in manganese, nutrient concentration prediction in surface water systems, with better accuracy than regression-based techniques]. Nevertheless, a large number of studies were concerned more with spatial prediction and did not pay much attention to the aspect of temporal forecast. This will diminish their real-world usefulness as a predictive approach and as a source of future-risk assessment. As a result of the emergence of deep learning, recurrent neural networks and long short-term memory networks started to become common in order to model the time-dependent nature of water quality time series. The LSTM models exhibited high performance when it comes to the long-term dynamics of nutrients, especially in the forecasting of nitrate within the low-frequency monitoring conditions. More stability and noise-reduced hybrid deep learning models that integrated empirical mode decomposition and LSTM enhanced each other. Multivariate LSTM allowed the concurrent prediction of many water quality parameters, and it has high generalization compared to univariate models [15]. Regardless of these benefits, deep learning models are large dataset-consuming, expensive to compute, and require hyperparameter optimization [24]. Additionally, most deep learning research concentrated on limited horizon forecasting and neglected the space.

This restricts their use in large-scale nutrient management and policy planning. The water quality processes are both spatiotemporal by nature, i.e., are not the same at both space and time [25]. Geospatial prediction models have been used to find nitrate concentration in groundwater and the most at-risk zones of contamination. These models helped in giving insight into land use management and agricultural policy. Residual chlorine, dissolved oxygen, and nitrate dynamics of river systems and water distributions have also been modeled using spatiotemporal models [26]. Through the combination of machine learning and hydraulic simulations, there was an increase in the spatial consistency and time accuracy. Recent research

on deep learning showed that watersheds, soil behavior, and discharge trends cause climatic variations to have significant impacts on the nitrate cycle. Nonetheless, the spatiotemporal models are yet to be applied in nutrient forecasting, especially in relation to both seasonal and long-range prediction [27]. One of the most predominant trends of nutrient time series is seasonality The cycles of applying fertilizers, rainfall fluctuations, the way irrigation is undertaken, and the level of biological activity develop robust periodic trends in the nitrate, ammonia, and orthophosphate levels. The omission of seasonal effects has been revealed to lead to substantial undercutting in the accuracy of the forecasts [28]. The use of periodical features and seasonal encoding has enhanced the performance of the model in a number of deep learning experiments. Nevertheless, a large number of current models continue to use the simple lag variables without modelling seasonal periodicity [29]. Water management requires seasonal forecasting because the risk of overload of nutrients is usually at certain months. Regardless of such importance, the major part of the literature currently is not focused on seasonality as an independent model element [30]. The concept of hybrid model strategies has also become an effective measure of enhancing predictive soundness. Hybrid models are frameworks that use machine learning models as well as deep learning models so that they can leverage their areas of strength [31]. Mechanisms Residual learning methods: Neural networks identify the machine learning errors and rectify them, leading to promising outcomes in environmental modeling. Comprehensive findings have been presented in Table 1.

Combination methods with several algorithms also have enhanced stability and generalization. Nevertheless, the hybrid methods are not very common when it comes to the nutrient forecasting applications [32]. The other significant drawback of the existing water quality modeling is the inability to quantify the uncertainty. Environmental risk management requires deterministic predictions, but confidence intervals are necessary in order to make regulatory decisions. Measurement error, variation in the environment, structure of the model, and lack of data are sources of uncertainty [33]. Nevertheless, point measures, including RMSE and R 2, are the most reported in most of the studies. To close this gap, the use of conformal prediction and probabilistic modelling has recently been suggested. Conformal prediction provides distribution-free uncertain estimation; hence it is especially applicable in ecological conditions [34]. Nevertheless, uncertainty-aware nutrient forecasting has not been done extensively at local and multisite levels.

Climatology and persistence are some of the common strategies of forecasting models on the baseline. Climatology is based on long-term averaging, whereas persistence assumes that future values are equal to the recent values [35]. Persistence is usually quite effective in short-term forecasting when there are sudden season changes or extreme events. Climatology is not very good when the interannual variability is high. Most of the studies do not operate the due comparison of the bases, causing excessive assertion of model performance. The scarcity of data also makes it hard to model nutrients. Most water quality datasets have gaps, sporadic time intervals, and a narrow history. In gap filling and interpolation, machine learning method has been used successfully, and little focus has been directed to finding out the role played by data density on long-term predictions [36]. Cost monitoring is an issue of concern, especially in developing areas. Predictive modeling is more cost-effective because it lessens the need to have thick monitoring networks but affords effective risk evaluation. But still, the combination of high accuracy, seasonality consistency, spatial generalization, as well as uncertainty reliability is an unsolved research problem. According to the literature reviewed, there are some gaps in the research. Current literature seldom incorporates spatial, temporal, and seasonal elements in a single nutrient prediction model. The use of uncertainty-aware modeling is still very far from being widely adopted in nutrient concentration prediction. Nutrient studies are under-researched in hybrid machine learning and deep learning. Extensive blindness on climatological and persistence baselines is not always available. In addition, the

three-way (nitrate, ammonia, and orthophosphate) are all too often not jointly modeled in the same framework. Such gaps suggest that there is a need to have a complete spatiotemporal seasonal nutrient forecasting model, which includes the quantification of uncertainty. This type of construct would greatly contribute to the enhancement of decision-making as far as the safety of drinking water, agricultural management, and the development of environmental policy are concerned.

**Methodology:**

This part explains how the data are prepared, how the features will be built, how the predictive model will be structured, how the uncertainties will be estimated, and how it will be evaluated, which will be implemented in seasonal spatio-temporal nutrient concentration forecasting. Figure 1 presents the methodology of the proposed work.

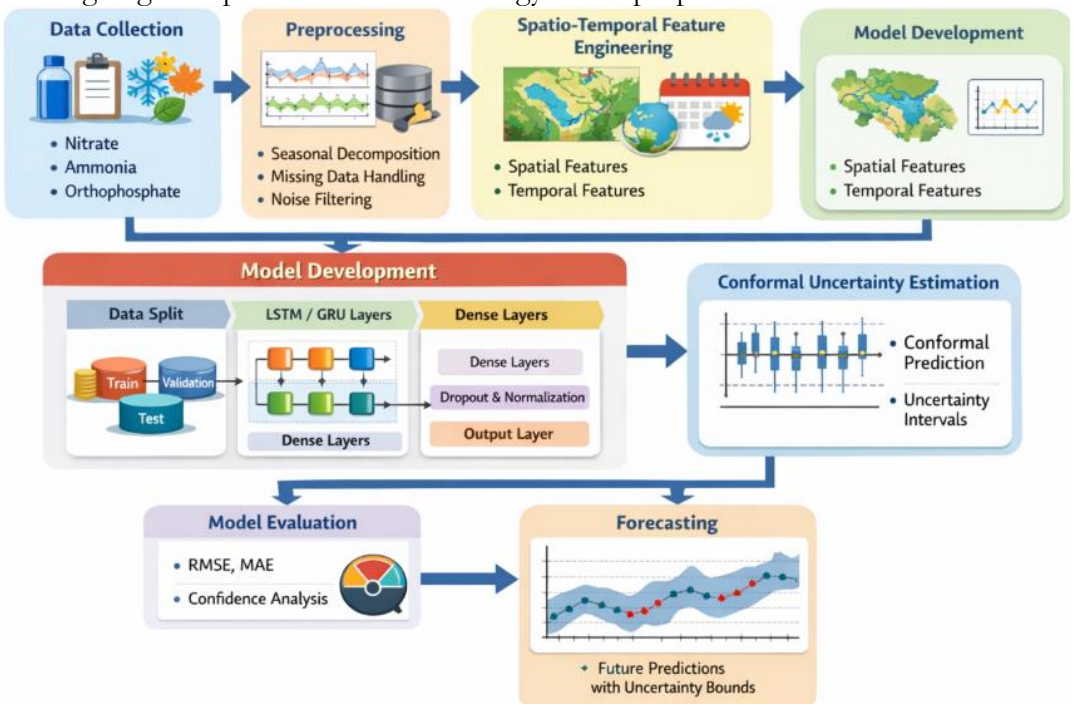


**Figure 1.** Methodology workflow diagram

**Selection of Data and Variables:**

California monitoring programs were the source of surfaced waters quality observations that were taken during the year 2010 through to 2025. The resulting merger dataset consisted of 293231 records along with 81 attributes, which reflected values of measurements of various monitoring locations spread across California surface water bodies. Three of the nutrients were chosen out of all the parameters available and were based on the environmental significance, relevance to regulations, and the availability of data:

Nitrate

Ammonia

Orthophosphate

The mentioned nutrients are considered the most important evidence of eutrophication, agricultural runoff, and water quality deterioration. Records that matched these three nutrients were therefore retained to be used in modeling.

**Table 1.** Literature Review Analysis

| Study | Water System | Focus / Nutrients | ML Application | Comments on Exploration |
|---|---|---|---|---|
| [1] | **Surface water (river)** | Nitrate, ammonia, turbidity, etc. | Hybrid regression + XGBoost to predict multiple water quality metrics, including nitrate & ammonia, across seasons. | Demonstrates recent ML application for surface water quality, but relatively few examples exist compared to traditional hydrogeochemical studies. |
| [17] | **Surface water (river network)** | Nitrate & orthophosphate | Random forest model trained on the river network graph to map seasonal nutrient distributions. | One of the few surface water nutrient ML studies indicates relevance, but still emerging. |
| [25] | **Surface water (river)** | General water quality indicators, including nitrate | Kernel extreme learning machine for classification/forecasting of river water quality. | Adds to the limited surface water ML forecasting literature; however, nutrient-specific forecasting ($NH_3$, $PO_4$) remains less frequent in broader ML studies. |
| [18] | **Groundwater** | Contamination generally (including nitrate) | Systematic review summarizing ML methods applied to groundwater monitoring/contamination prediction. | Highlights more widespread ML applications in groundwater environmental monitoring, albeit not exclusively nutrient forecasting; suggests broader interest and adoption in groundwater research. |
| [19] | **Groundwater** | Nitrate | Multiple ML algorithms to model shallow groundwater nitrate variability. | Example of focused groundwater nutrient (nitrate) ML modeling, showing multiple algorithm comparisons—an established niche relative to surface water. |

**Data Cleaning and Reduction:**

To enhance the reliability of the data, several preprocessing procedures were used:
Records containing gaps of non-numeric and negative concentration values were eliminated.
Measurements of duplicate dates on websites were filtered.
The dates of sampling were transformed into temporal attributes.
Valid surface water sampling sites only were maintained.

The dataset was narrowed down to 259,703 valid records with 6 core attributes of site identifier, sampling date, nutrient type, value of concentration, year, and month following the cleaning.

**Temporal Aggregation:**

Since the frequencies of sample differed at different sites, monthly aggregation was used. On every site and nutrient, average measurements within a given month were calculated to get a consistent monthly time series.

In this aggregation, 60,125 spatio-temporal samples were generated, which ascertained a regularity in time while conserving the long-term seasonal processes.

**Feature Engineering:**

The seasonality was coded as cyclic transformations:
Sine and cosine functions were used to express the month, as it was a periodic number.
The year was considered to obtain the long-term temporal trends.

The identity of nutrients was numbered, and as such, nutrient-specific behavior could be learnt. Site sampling frequency was used in approximating spatial influence.
It included temporal dependency features, Lag-based:
concretion of previous month (Lag-1).
Three months earlier concentration (lag-3).
Rolling Mean over 3 months.
Rolling standard deviation over 3 months.

These aspects enable the models to possess persistence, delayed responses, and the short-term variability.

Due to the lag and rolling properties, 15,881 records were dropped to leave the final modeling data of 44,244 samples and 9 predictive features.

**Dataset Partitioning:**

The time-ordered split was used to ensure that no future information is leaked:
80% for training.
20% for testing

**Baseline Forecasting Techniques:**

Two basic baselines were put in place:
**Persistence baseline**: which assumes the next value equals the most recent observation.
**Climatology baseline**: which uses the long-term monthly median concentration.
These baselines are typical assumptions of operation forecasting and are used as a norm by which the improvement of models can be compared.

**Predictive Models:**

The reason behind the choice of three machine learning models was their complementary strengths.

Random Forest regression consists of a collection of decision trees that are trained on random sets of data and features. This architecture allows effective acquisition of nonlinearity about the relationships and smoothing overfitting by averaging.

XGBoost regression uses gradient boosting in order to enhance predictive accuracy. Every tree removes the orphan errors of the former trees, which results in a great predictive precision and high generalization.

**Random Forest Neural Network Model Hybrid:**

A hybrid structure was developed based on Random Forest with the aid of a feed-forward neural network. The initial predictions were generated by the use of random Forest. The remaining errors between the predictions and observations were modeled, then, with the help of a neural network. At the end of the forecasts generated using the Random Forest were added to the previously generated neural network residual prediction to provide the final forecasts.

This architecture enables the ensemble learning to acquire the overriding patterns, and deep learning concentrates on the overriding nonlinear residual structures.

**Conformal Prediction-Based Estimation of Uncertainty:**

Conformal prediction was used to measure prediction uncertainty. Non-conformity scores were computed with the help of residuals of the calibration dataset. Symmetric 90% prediction intervals around model forecasts were then made by using these scores.

Conformal prediction ensures valid coverage without the assumption of a probability distribution since it applies to data in the environment in which the noise has heterogeneous properties.

**Evaluation Criteria:**

Assessment of model performance was done using:
Mean Absolute Error (MAE)
Root Mean Square Error (RMSE)
Coefficient of Determination ($R^2$)
The probability of prediction interval coverage.
Average interval width
These measures are a combination of point accuracy and uncertainty reliability.

**Experiments and Results:**

This part will outline the experiment setup, the nature of the databases, and the relative forecasting results of the suggested nutrient concentration prediction model. Three key nutrients, Nitrate, Ammonia, and Orthophosphate, are assessed, but consider the seasonal spatio-temporal characteristics and uncertainty-based prediction.

**Experimental Setup:**

They were performed with the help of standard machine learning and deep learning libraries. The design makes reproducibility and fair comparison of models
The following are the software specifications:

| Component | Specification |
|---|---|
| Platform | Google Colab (Cloud-based Jupyter Notebook) |
| Programming Language | Python 3 |
| Deep Learning Framework | TensorFlow / Keras |
| Machine Learning Libraries | Scikit-learn, XGBoost |
| Data Processing | Pandas, NumPy |
| Visualization | Matplotlib, Seaborn |
| Uncertainty Modeling | Conformal Prediction implementation |
| Operating System | Managed by Google Colab (not locally installed) |

The following are the Hardware specification:

| Component | Specification |
|---|---|
| CPU | Intel Xeon (virtualized) |
| GPU | NVIDIA Tesla T4 |
| RAM | 16 GB |
| Storage | Cloud-based virtual storage |

**Dataset Description:**

This data was collected from the California Surface Water Quality Monitoring Programs for the time period of 2010 to 2025.

The analysis focused on:

Nitrate

Ammonia

Orthophosphate

These nutrients are widely regarded as major contributors to eutrophication and degradation of surface water quality [1][8][3][4].

| Attribute | Description |
|---|---|
| Study Area | California, USA |
| Water Type | Surface Water |
| Time Span | 2010 – 2025 |
| Temporal Resolution | Monthly |
| Nutrients | Nitrate, Ammonia, Orthophosphate |
| Initial Records | 60,125 |
| Records after Cleaning & Feature Engineering | 41,847 |
| Sites | 5,380 |
| Features Used | Year, Seasonal Encoding, Nutrient Code, Site Frequency, Lagged Values, Rolling Statistics |
| Target Variable | Nutrient concentration |
| Data source | California open data portal: https://data.ca.gov/ |

**Results:**

Three similar nutrients, including Ammonia, Nitrate, and Orthophosphate, that had been extracted out of long-term monitoring records spanning between January 2010 and October 2025, were used to test the suggested spatio-temporal nutrient forecasting structure. The last nutrient data set was a processed data set with 128,531 valid observations of 4,977 monitoring locations. Aggregation into discrete records per month created 54999 records, with 41847 samples left following lagged entity engineering, rolling window engineer-rolled window features, which is a reduction in the data by 23.9%. The last dataset was further cut into training (33477 samples), calibration (4185 samples), and testing (4185 samples) datasets to prevent information leakage due to time.

**Table 2:** Performance Comparison of Nutrient Forecasting Models

| Model | MAE | RMSE | $R^2$ | Coverage (90%) | Avg. Interval Width |
|---|---|---|---|---|---|
| Random Forest + Conformal | 0.100847 | 0.229443 | 0.774574 | 0.881243 | 0.395502 |
| Hybrid (RF + FNN Residual) + Conformal | 0.101008 | 0.229414 | 0.774633 | 0.894863 | 0.432019 |
| XGBoost + Conformal | 0.115224 | 0.243795 | 0.745493 | 0.878853 | 0.453779 |
| FNN + Conformal | 0.142401 | 0.268205 | 0.691976 | 0.879809 | 0.534485 |
| Persistence Baseline | 0.175692 | 0.414440 | 0.264514 | nan | nan |
| Climatology Baseline | 0.335974 | 0.569476 | 0.388684 | nan | nan |

Table 2 shows the comparative results of all of the considered models in the form of Mean Absolute Error (MAE), Root Mean Square Error (RMSE), coefficient of determination (R2), and conformal prediction interval reliability. Of all models, the Random Forest with Conformal Prediction had the lowest MAE of 0.1008 and the lowest RMSE of 0.2294, which means that it has high predictive capabilities and good consistency. A similar result was obtained with the Hybrid Random Forest + Neural Network model, with an MAE of 0.1010 and RMSE of 0.2294, which indicates that the residual learning did not indicate any appreciable difference from the baseline of the Random Forest.

The XGBoost model was a bit less accurate with an MAE of 0.1152 and R2 of 0.7455 as compared to feed forward neural network, which portrayed lower performance with an MAE of 0.1424 and R2 of 0.6920. The results of both baseline methods, such as persistence and climatology, were significantly worse, thus reaffirming the need to have more sophisticated machine learning models to predict nutrients in complex environmental systems.

Conformal prediction as a method of quantifying uncertainty was found to be reliable, covering all the learning models. The hybrid model has the highest probability of 0.8949, which has a coverage of 90%, and then in figure5, there were the probabilities of Random Forest and XGBoost of 0.8812 and 0.8789, respectively. As much as the Hybrid model (figure 4) generated relatively wider prediction sets as compared to the Random Forest (Figure 2), the enhanced coverage implies enhanced reliability of uncertainty. A feed-forward neural network (Figure 3) produced the widest intervals because there is greater uncertainty of prediction as it has lower accuracy.

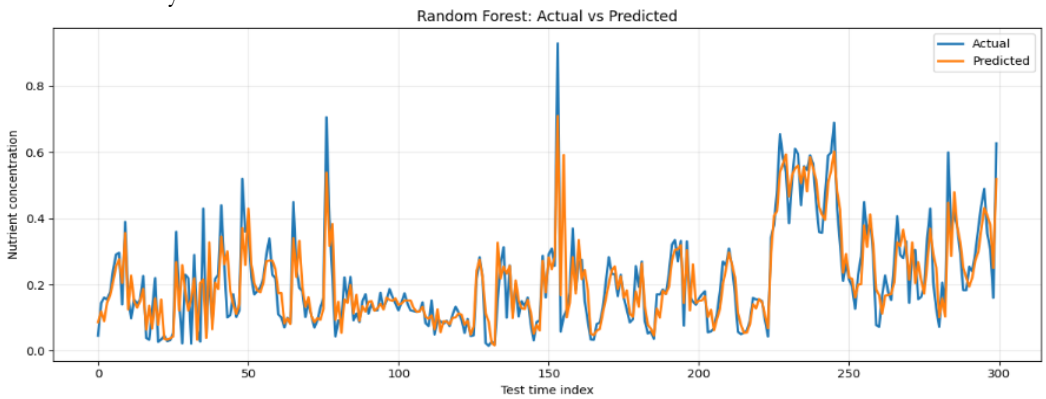


**Figure 2.** Random Forest actual vs predicted

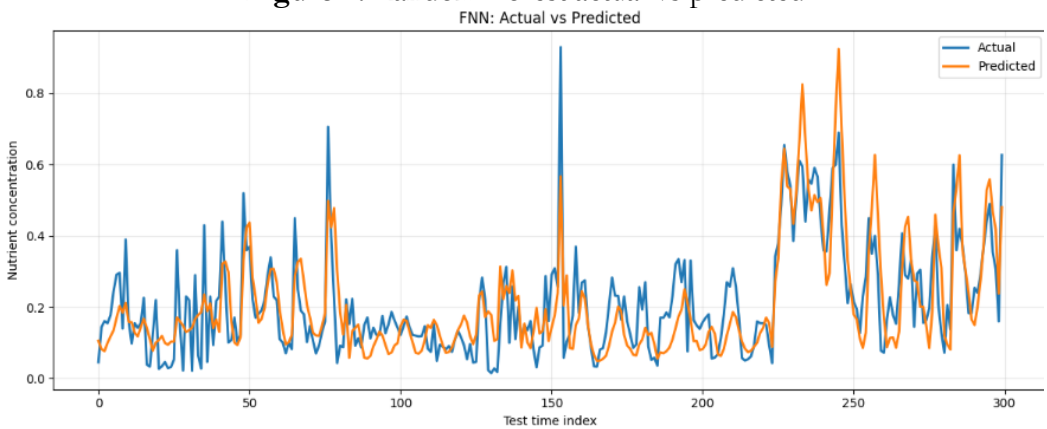


**Figure 3.** FNN actual vs predicted

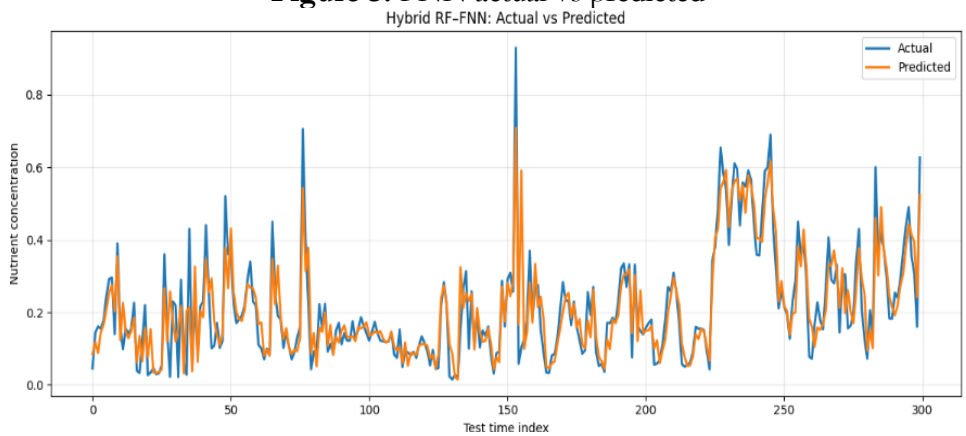


**Figure 4.** Hybrid (RF + FNN) actual vs predicted

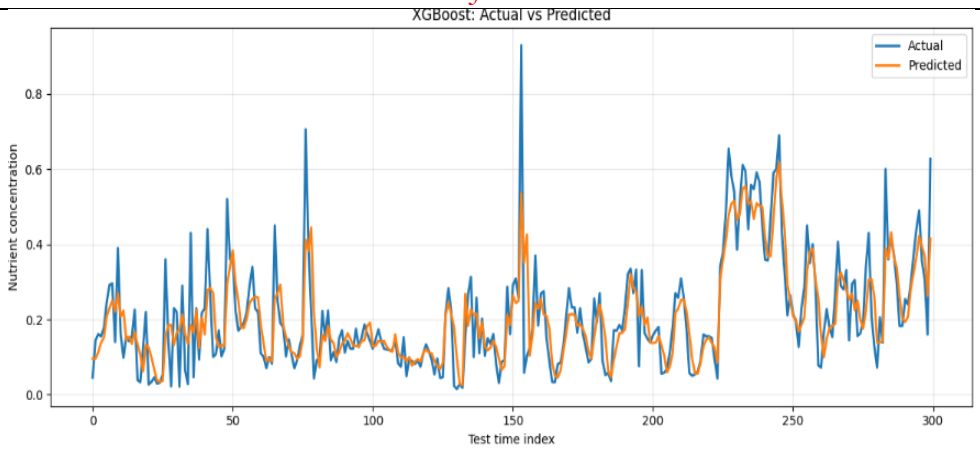


**Figure 5.** XGBoost actual vs predicted

The best performing random forest model results in changing the actual and predicted nutrient concentrations, as seen in figure 6. The observed values are close to the predicted ones, with only a slight deviation, as most time intervals are concerned. The conformal prediction bands that were associated achieved success in encapsulating most of the observed concentrations, indicating sound uncertainty calibration.

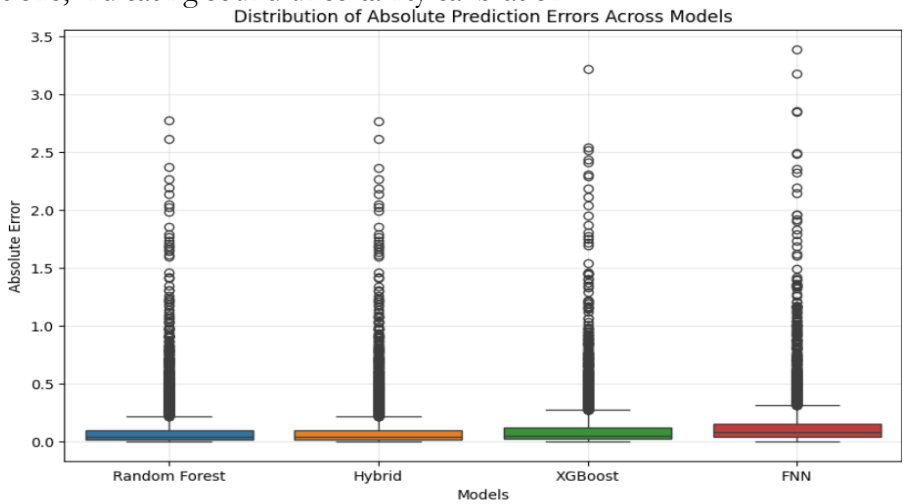


**Figure 6.** One-Way ANOVA Comparison of Prediction Errors Across Forecasting Models

The absolute prediction errors were subjected to one-way analysis of variance (ANOVA) to statistically prove that there were differences between the performances of the models (Figure 6). The F-statistic has been provided, which is 35.02 with a p-value of 1.50x10-22 resulting in a negative value and showing that there is no significant difference in all the model performances. The corresponding boxplot of the error distribution further explains the fact that the median errors and dispersion of the Random Forest and the Hybrid models are always lower than those of the XGBoost and neural network models.

All in all, the findings support the assertion that ensemble tree-based learning, especially Random Forest with confirmed uncertainty estimation, is the most robust and predictable model with regard to the forecasting of seasonal spatio-temporal nutrient values. The hybrid residual learning approach also provides more reliable uncertainty, but does not significantly exceed the Random Forest in the accuracy of point prediction. The results show that ensemble learning with distribution-free uncertainty quantification is appropriate in the operational assessment of water quality and early estimation of the risk of contamination.

**Discussion:**

The findings show that the use of ensemble-based model together with conformal prediction gives sound and effective nutrient concentration predictions. RF + FNN residual

+ Conformal and Hybrid models showed the lowest errors in prediction and the largest power of explanations, which proves the good generalization ability of such models in monitoring sites with heterogeneity. Conformal prediction was successfully used to control the reliability of the prediction by making sure that about 90 percent of the observed values fell within the uncertainty intervals, and thus, valid error control was done without distribution assumption.

The hybrid residual learning method also enhanced the coverage of uncertainties by processing systematic errors of the Random Forest with a neural network, but retained the robustness of an ensemble at the same time. Conversely, the standalone neural network exhibited lower stability as well as greater error prediction, which indicates that it is sensitive to noise and low temporal structure in environmental data. Very poor performance was seen in the case of baseline persistence and climatology models, and thus, it is clear that the advanced machine learning methods are required in nutrient dynamics. To validate statistically that there were significant differences between the performance of models, ANOVA was used, which confirmed that the differences between the models were significant ($p < 0.001$), further lending credibility to the comparison. In general, the suggested framework manages to balance predictive accuracy with uncertainty reliability, thus qualifying to be used in both the operational water quality monitoring and decision support applications.

**Limitations and Future Work:**

Despite the high predictive power of the suggested framework of nutrient forecasting in seasonality and a solid uncertainty estimate, one must admit a number of limitations. To begin with, monthly aggregated observations would smooth the short-term variation and extreme cases of pollution, which are significant to early warning and rapid response potentials. Faster dynamic processes of nutrients might be captured by the daily or weekly data. Second, the models that are developed strongly depend on the tariffs of nutrients in the past. In cases where the monitoring stations have some missing records or long intervals, the reliability of the prediction can be low, although there is preprocessing work done. Third, spatial interaction between monitoring locations had no explicit model. The nutrient transfer is highly affected by the hydrological connectivity, the discharges upstream, and the watershed properties. The fact that these spatial dependencies can be ignored will limit the possible capacity to explore nutrient movement across regions completely. Fourth, conformal prediction methodology is the assumption that the methods of calculating the prediction are similar in the cases of calibration and the test samples. This assumption can be compromised under climate variability, any change in land use, or some regulatory interventions, which can influence uncertainty coverage. Then, in future studies, better temporal resolution data sets may be utilized so that they can perform better at short-term forecasting. Graph neural networks or geostatistical models of spatial learning can be combined to learn watershed connectivity. Model generalization can also be enhanced by the use of additional environmental drivers such as rainfall, discharge, temperature, and land use indicators. In addition, multivariate nutrient forecasting and adaptive conformal methods are some of the areas that can be investigated in a bid to enhance the reliability of uncertainty in non-stationary circumstances. Such enhancements are able to promote better reading, inferential, and operationally feasible nutrient observing frameworks of water quality administration.

**Conclusion:**

Spatio-temporal prediction of nutrients at the seasonal level is necessary in managing water resources sustainably and in early warnings of contamination risks. The suggested framework has proven that the idea of using machine learning along with uncertainty quantification can be useful in modeling the dynamics of nutrients in large-scale monitoring databases. Random Forest, XGBoost, feed-forward neural networks, and residual hybrid strategy were all successfully used to predict monthly nutrient concentrations of nitrate, ammonia, and orthophosphate. Random Forest-based and conformal prediction had the best

combination of both in terms of accuracy and uncertainty reliability, and so does the hybrid residual model. These findings affirm that ensemble learning techniques are very strong in terms of tabular environmental time series data, and neural networks add some value to tabular environmental time series data when they are used to clean up the residues. The addition of conformal prediction allowed predicting statistically valid intervals of prediction, which give useful confidence limits that are indispensable in the context of environmental decision-making. Persistence and climatology-based baseline methods indicated significantly less responsive results of the nonlinear seasonal and temporal nutrient patterns, enhancing the usage of complex machine learning models. The ANOVA method of statistical test also established that the performance variances exhibited between the models were statistically significant, which supported the credibility of the comparative analysis. In general, the framework developed offers an interpretable and scalable solution that is uncertainty-aware in terms of nutrient concentration prediction. The findings reveal that it has great potential to be used in water quality control, regulation control, and risk-based resource control. The framework allows for better-informed environmental planning by balancing predictive performance with uncertainty disclosure, which leads to the further accomplishment of safer and more sustainable water systems.

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