Exploring AI Techniques for Effective Monitoring of Aquatic Toxicity

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Abstract

The quality of water has an impact on both the environment and human health, so this makes the monitoring of water quality crucial. This research aims to explore the applications and benefits of Artificial Intelligence (AI) in this topic by presenting some examples of usages in real scenarios and analyzing the status of the research conducted in this context using neural network models. We will show that Back Propagation Neural Network (BPNN), Adaptive Neuro-Fuzzy Inference System (ANFIS) and Artificial Neural Network (ANN) have been the most commonly used neural network technologies in the last ten years. Despite the first one is the most popular, by evaluating the relation between frequency of model usage and their R^2 result, it is clear that ANN and ANFIS are likely the most useful models for data predictions in water quality monitoring.

Introduction

Water is fundamental for life. It covers 71% of the earth by considering oceans, rivers, lakes, icecaps and glaciers. Thus, its quality impacts on the

- environment: ecosystems rely on a complex web of animals, plants, bacteria, and fungi—all of which interact with each other. Harm to any of these organisms can create a chain effect, imperiling entire aquatic environments;
- human health: 1 billion people fall ill every year from unsafe water.

Monitoring water quality is therefore crucial and, nowadays, it is done by sampling the chemical condition, sediments and fish tissue to determine levels of key constituents and by monitoring physical conditions such as temperature. Also, biological measurements of the abundance and variety of aquatic flora and fauna are used. Nevertheless, these approaches could have many limitations, such as the cost, the time needed and the ethics regarding the use of animals. Also, it would be better to predict water quality in order to mitigate the effects quickly and prevent the causes.

In this scenario, Artificial Intelligence systems could be very useful because they permit a real-time analysis, early detection of toxic events and efficient identification of toxic substances and their sources.

In this paper, we would like to:

- stress the importance of monitoring the water;
- demonstrate how AI models could be useful in this theme by showing some examples of usages in real scenarios;
- present the status of the research conducted in this area by updating the paper publish by Singh et al.(Singh, Gupta, and Rai 2013) with new studies.

Water quality and its social impact

Water quality monitoring, and in general, management is among the most important elements to achieve a sustainable future in the next years. It requires interdisciplinary efforts that encompass various key aspects including:

- wildlife and biodiversity conservation
- managing environmental issues
- economic concerns
- societal well-being

Water quality management initiatives, indeed, have a direct impact on wildlife preservation and biodiversity conservation. By maintaining and improving water quality, we create healthier ecosystems that support the growth of healthy flora and fauna. Clean water bodies provide habitats for aquatic organisms and contribute to the overall balance of ecosystems. Preserving biodiversity is not only important for the intrinsic value of the natural world but also for the ecological services they provide, such as pollination, nutrient cycling, and disease control.

Environmental issues are closely linked with water quality management. In facts, contamination of water sources by pollutants, such as industrial waste and agricultural runoff, as we will see in later chapters, poses significant threats to both human health and the environment. By implementing effective water quality management strategies guided through effective monitoring, we can mitigate the pollution of water bodies, protect sensitive ecosystems, and ensure the availability of safe drinking water for communities. This, eventually, reduces the risk of waterborne diseases and enhances public health.

Water quality management also has economic implications. Clean water is essential for industries such as agriculture, manufacturing, and tourism. By maintaining high water quality standards, we safeguard the productivity of agricultural lands, protect the integrity of industrial processes, and attract tourists to appealing and safe water bodies. Moreover, a healthy environment supported by water quality management measures helps sustainable economic growth, as businesses can thrive in a clean and attractive setting.

Societal issues are deeply interconnected with water quality management. Access to clean water is a basic human right, and communities that lack safe drinking water face significant social and health challenges. By ensuring water quality, we address social equity and empower vulnerable populations. It is now common knowledge, the power to subjugate entire populations with the threat of removing this essential element can lead to instability and oppression.

So we just shown that the social impact of water quality management extends beyond environmental concerns. It's our aim to discuss and analyze how artificial intelligence can help, mainly through monitoring, to manage this task.

Different usages of AI models in real scenarios

In this section, we will go through some papers to have a close look at how AI can be applied in real scenarios of water quality. We will discuss the benefits and results of these applications. Specifically, we will discuss four different applications showcased in four different papers that effectively utilize four distinct AI techniques to achieve their goals in various water quality scenarios. These four papers were selected because they provide diverse real-life examples.

Water treatment for optimization and automation of adsorption processes

Access to clean drinking water is the grand challenge of the modern era, but water pollution caused by rapid industrialization and population growth has emerged as a grand environmental challenge in recent years. Treatment and reuse of wastewater offer a unique opportunity to address both these challenges. AI is expected to save 20 to 30% of operational expenditures by decreasing the cost and optimizing the usage of the chemicals in water treatment. Various studies demonstrated the successful applications of different AI for modelling and optimization of the water treatment process. While analyzing different AI tools they compare the performance of the adsorption process employed for the removal of metals, dyes, organic compounds, nutrients, pharmaceuticals, drugs, pesticides, and personal care products (PCPs) from the water.

AI techniques

- k-Nearest Neighbor (k-NN)
- Decision Tree (DT)
- Random Forest (RF)
- Artificial Neural Networks (ANNs)
  - Fuzzy Neural Network (FNN)
  - Convoluted Neural Network (CNN)
  - Deep Neural Network (DNN)
  - Recurrent Neural Network (RNN)
- Support Vector Machine (SVM)
- Self-Organizing Map (SOM)
- Genetic Algorithm (GA)
- Particle Swarm Optimization (PSO)
- AI hybrid techniques

Applications of AI tools in water treatment AI techniques were effective in establishing a relationship between the various variables in water treatment process. Some studies also predicted the simultaneous removal of multi-pollutants from the water with the aid of AI improving the efficiency of real water treatment systems.

- Removal of dyes
- Removal of heavy metals
- Removal of organic compounds, nutrients, pharmaceuticals, drugs, pesticides, and PCPs from the aqueous phase
- Applications of hybrid techniques in water treatment

In general, hybrid techniques were more effective in predicting process performance as compared to individual techniques.

Challenges and prospects AI tools can be used to predict the performance of various water treatment process and reduce the experimental costs. The major drawback of the ANNs group is the poor reproducibility due to the random weight and bias that might result in local optimal solution. Deep ANNs are good options for achieving high accuracy and prediction, but requires sufficient amount of data. The process performance predicted by AI tools may also deviate from the actual results under certain circumstances. Another challenge is the availability and selection of data to be computed (special care should be taken while collecting the data to keep data integrity). AI technology could play a critical role in sustainable wastewater treatment and can result in a significant reduction in operating cost in addition to safeguarding the environment. By applying hybrid AI techniques, prediction accuracy can be enhanced that leads to a reduction in energy and operational cost.

Conclusion The current research progress suggests that AI tools have a bright future in water treatment applications. (Alam et al. 2022)

Aquatic toxic analysis by monitoring fish behavior

Monitoring aquatic toxicity is a fundamental and essential task for risk assessment in aquatic ecosystems and water resource management. Physicochemical parameters are widely adopted, but the sensors could only detect known toxicants within a period.

Behavioral monitoring uses instead the responses of indicator species to the surrounding environment. The latter is an efficient approach for long-term monitoring since the accumulation effects of disturbance or chemical stress could be relevant by behavioral monitoring. Fish and daphnia are the common indicator species due to their sensitivity to changes.

In the early stage of behavioral monitoring of aquatic organisms, behavioral signal was represented by the strength of electrical fields. With the advent of computer vision we instead track single individual or multiple individual in 2D and 3D space, becoming the common tool for obtaining behavioral data.

Deep learning recently brings strong influence, but it is still in the starting stage for toxicity prediction.

Video Tracking Based Behavioral Monitoring Monitoring individuals could reveal behavioral changes, as they are more sensitive to toxic and pollution. CV based biological monitoring achieved great attention since many observation systems were developed and behavioral sensing has been studied for determining aquatic toxicity. Individual organisms are detected and located using image processing and tracking algorithms (video analysis), but this practice requires extreme large amount of storage and is not suitable for long-term behavioral monitoring. Instead, real-time behavioral observation is adopted for immediate examining data from observation area. The pros of this approach is that we detect environmental risks at early stages and for long-term observation we can store data in text files or databases, cons is that it requires hardware and high performance and efficient algorithms to process video stream from live camera data.

For tracking there are two approaches:

- Two-dimensional tracking
- Three-dimensional tracking

Toxic analysis The water quality monitoring technique on the basis of behavior changes of aquatic organisms is an advanced technique in the field of monitoring water environment change. It possesses the characteristics such as high stability and reliability, easy maintenance, and low operating cost. The behavioral indicator includes escape, motor and breathing behavior.

Conclusions Rapidly developed machine learning algorithms are superior in predicting aquatic toxicity. However, video tracking based toxicity sensing is still in its initial stage and one important issue to be solved is the computational expensive operations involved for real-time data analysis. (Xia et al. 2018)

Models for Accurate Estimation of Groundwater Nitrate Concentration

Groundwater nitrate concentration prediction is essential for managing water resources in arid regions. Increased population, climate change, and agricultural practices contribute to nitrate pollution. This research focuses on modeling nitrate concentration using artificial intelligence in the Marvdasht watershed, Iran. The aim is to aid in managing and improving groundwater quality.

Materials and Methods

- AI moldes: in this study are evaluated four different model: Cubist, SVM, RF, and Baysian-NN
- Dataset: groundwater-nitrate concentrations were provided by the Iranian Department of Water Resources Management (IDWRM) at 67 wells during June 2018.
- Features used: various influential geo-environmental variables on nitrate concentration were assembled for the case study: elevation (m), slope (%), plan curvature, profile curvature, annual rainfall (mm), piezometric depth (m), distance from residential (m), distance from the river (m), (Sodium) Na (mg/L), (Potassium) K (mg/L), and TWI.
- Evaluation tools: as evaluation tools were used R^2 coefficient of determination, the Root Mean Square Error (RMSE),the mean absolute error (MAE) and the Nash–Sutcliffe model efficiency coefficient(NSE).

Results the result shows how RF model (R^2 , 0.89; RMSE, 4.24; MAE, 3.55; NSE, 0.87) is capable of providing the best results compared to the Cubist and the other three models.

Model	Stage	R^2	RMSE	MAE	NSE
Cubist	Training	0.96	3.52	2.52	0.95
Cubist	Validation	0.87	5.18	4.06	0.81
SVM	Training	0.94	4.24	2.73	0.94
SVM	Validation	0.74	6.07	5.07	0.74
RF	Training	0.96	3.66	2.72	0.95
RF	Validation	0.89	4.24	3.55	0.87
B. ANN	Training	0.88	5.89	4.56	0.88
B. ANN	Validation	0.79	5.91	4.67	0.7

Conclusion Due to agricultural development and human activities, the average amount of nitrate in groundwater bodies has been increasing in recent years, polluting them. As part of this research, four different machine learning models were employed to predict nitrate pollution in the Marvdasht plain of Fars Province. The results of the ML models demonstrated their capability to predict nitrate pollution in groundwater. Specifically, the RF model with NSE = 0.87 outperformed the other three models. Moreover, it was found that nitrate contamination is more pronounced in the northern parts of the watershed, likely due to mismanagement of wastewater and chemical fertilizers. To address this issue, regular monitoring of groundwater and the education of farmers can play a crucial role in preventing excessive pollution and safeguarding water resources. (Band et al. 2020)

Predicting acute aquatic toxicity of structurally diverse chemicals in fish using artificial intelligence approaches

Every day, various synthetic chemicals are added to the existing ones and some of them have been identified as potentially toxic. An appropriate tool for evaluating the safety of organic chemicals is the medial lethal concentration (LC_{50}) test. Nevertheless, this experimental approach has many limitations, such as the cost, the time needed and the ethics regarding the use of animals. To overcome these issues, it is fundamental to predict the toxicities of the chemicals and the Artificial Intelligence (AI) approaches are particularly useful for capturing the complex non-linear relationships between the relevant properties and observed responses, as the structural properties used as estimators may have complex non-linear dependencies. Moreover, these models do not require knowledge of mechanisms and specific molecular descriptors derived from the chemical's structure. Several AI models were thus constructed for predicting the toxicity of the diverse chemical compounds using eight simple molecular descriptors . The compounds were classified into two classes (toxic and non-toxic) based on the EEC criteria and four classes (very toxic, toxic, harmful and not harmful) according to the European Community legislation. In the end, the models were evaluated and compared to each other.

AI techniques

- Probabilistic neural networks (PNNs)
- Generalized regression neural networks (GRNN)
- Multilayer perceptron network (MLPN)
- Radial basis function network (RBFN)
- Support vector machines (SVMs)
- Gene expression programming (GEP)
- Decision tree (DT)

Objectives, models development and evaluation The main objectives were to construct probability function-based neural network models (PNN and GRNN) and compared them with other nonlinear AI-based models (MLPN, RBFN, SVM, GEP, DT). Classification and regression models were developed to predict toxicity classes and acute toxicity (-log LC_{50}) of different chemicals using a selected set of properties/descriptors as predictors. For developing the models, different datasets were considered, such as the fathead minnow database (EPA) and other different data sources pertaining to different fish species for understanding if the models are appropriate for working well in noisy environments, like in the case of toxicity prediction of new chemicals. The selection of initial features involved two approaches: correlative and model-fitting. Descriptors with low correlation (less than 0.1) with the dependent variable were excluded. Nonlinear modeling was then performed using the PNN and GRNN approaches, trained with a Gaussian kernel function for measuring the similarity between the data. For selecting the optimal architecture of the models and to avoid overfitting, a ten-fold CV method was used during the training process. The classification models were evaluated based on the counts of true positive (TP), true negative (TN), false positive (FP) and false negative (FN) and the performance were assessed in terms of the misclassification rate (MR), sensitivity, specificity and accuracy of prediction. The performance of the regression models was evaluated using mean absolute error (MAE), root mean square error (RMSE), standard error of prediction (SEP), bias, the correlation coefficient (R) and the Nash-Sutcliffe coefficient of efficiency (E_f).

Conclusion The results suggest that the model for regulatory purposes should have high sensitivity, indicating its ability to recognize the toxicity of various compounds and high specificity, indicating its ability to recognize FP compounds. All the models achieved good performance, with PNN performing relatively better in classification and GRNN in the regression task. The PNN and GRNN models were tested with external datasets, and they performed well. This suggests they are appropriate for acute toxicity prediction of new chemicals and can be used as effective tools in regulatory toxicology decision making. (Singh, Gupta, and Rai 2013)

A wide overview of the state of art: Update analysis

Building upon the work presented in the study titled "Artificial Intelligence for Surface Water Quality Monitoring and Assessment: A Systematic Literature Analysis," our primary objective is to present an updated analysis of the research conducted in the field of surface water quality assessment using neural network models. The motivation behind undertaking this analysis is to analyze the subject from a comprehensive perspective and engage in an in-depth discussion on this important theme. By updating and comment the aforementioned study, we aim to contribute to the current understanding of surface water quality monitoring using AI models. Our analysis was conducted on a broad range of research studying this topic, with a specific focus on the utilization of neural network models. This approach allows us to examine the latest advancements, emerging trends, and significant outcomes in this field, ensuring that our discussion look at the subject also form a wide perspective.

Data and Analysis of literature To compile the literature for this review, a comprehensive search was conducted using the Web of Science (WoS) and/or SCOPUS databases. The search keywords used were "water quality," "artificial intelligence," and "surface water." Only studies specifically related to surface water were included, while papers on groundwater or rainwater were excluded. In contrast to the previous study, which included different elements, this update focused solely on the R^2 values, publication dates, and the neural network models utilized in the respective studies. In our work, our aim is to provide a partial update to the existing research. Conducting a rigorous and comprehensive update would be to much labor-intensive and time-consuming. Therefore, we have chosen to focus on updating specific aspects of the study to provide a more current analysis. The tables and charts were generated using Microsoft Excel ©2016 software in conjunction with Google Sheets. The additional data to update the paper are reported in Table 1.

Results of literature analysis

Model utilisation In this section, we will discuss the neural network model utilized in water quality monitoring and assessment. Looking at Figure 1, we can see that the number of published papers per year has stayed about the same over the past ten years. However, in the last two years, there has been an increase in studies, suggesting a possible change in research interests. However, we will later discuss that this increase doesn't necessarily mean better results. The consistent number of papers published may be caused there haven't been any groundbreaking discoveries in using neural networks for water quality assessment during this time, highlighting that this field is still relatively new. Looking at Figure 2, we can see that Back Propagation Neural Network (BPNN), Adaptive Neuro-Fuzzy Inference System (ANFIS), and Artificial Neural Networks (ANN) have

Table 1: Added data to the previous study

Year	AI model	R^2	Reference
2023	STHNT	0.911	(Ramaraj and Sivakumar 2023)
2022	PNN	0.94	(MF et al. 2022)
	CNN	0.87	(Pyo et al. 2022)
	ANN	0.949	(Ghasemi et al. 2022)
	ANN	0.82	(Arab et al. 2022)
	ANN	0.97	(Panahi, Mastouri, and Shabanlou 2022)
	PNN	0.93	(Allawi et al. 2022)
	ANN	0.93	(Aalipour et al. 2022)
	RBF-NN	0.989	(Egbueri and Agbasi 2022)
	MLP	0.987	(Egbueri and Agbasi 2022)
2021	ANN	0.94	(MI et al. 2021)
	ANN	0.99	(KJ, N, and NP 2021)
	GPR	0.987	(Ewusi, Ahenkorah, and Aikins 2021)
	MPL	0.989383	(Setshedi, Mutingwende, and Ngqwala 2021)
	W - ANN	0.9673	(Jamei et al. 2021)
	BPNN	0.913	(Ewusi, Ahenkorah, and Aikins 2021)

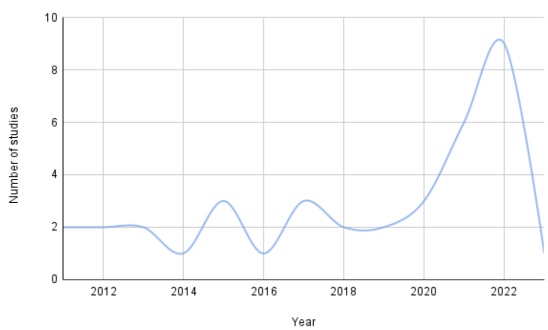

Figure 1: The number of studies for each year

been the most commonly used neural network technologies for monitoring and assessing water quality in the past ten years. Surprisingly, in contrast to the previous analysis proposed in the paper of Joshua O. Ighalo, BPNN turned out to be the most popular model, accounting for 20% of the total usage. This finding highlights the need for further research and development in this field, as these models were not originally designed specifically for water quality assessment. It is also important to note that BPNN, ANFIS, and ANN are not only the most frequently utilized models but also considered among the most common and easiest to implement.

Model accuracy In this analysis, we only considered studies that reported the coefficient of determination. We did not use the root mean square error (RMSE) because it is difficult to compare it directly across different parameters. The value of RMSE can vary greatly depending on the nature of the parameter itself. Parameters with large numeric values would tend to have larger RMSE values, but this doesn't necessarily indicate poor accuracy. Therefore, RMSE is not suitable for comparing accuracy across different parameters. Instead, we focused on the coefficient of determination (R^2) as a measure of accuracy. R^2 represents the extent to which the model captures the variability of the data. It ranges from 0 to 1, with 1 being the best possible value indicating a perfect fit to the data. We chose R^2 as it provides a simple and widely accepted measure for comparing accuracy in this study.

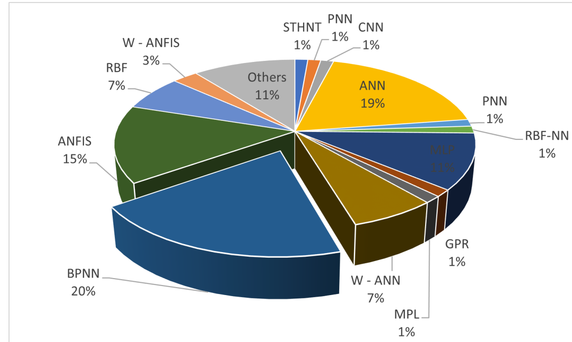

Figure 2: Frequency of application of neural networks in WQA

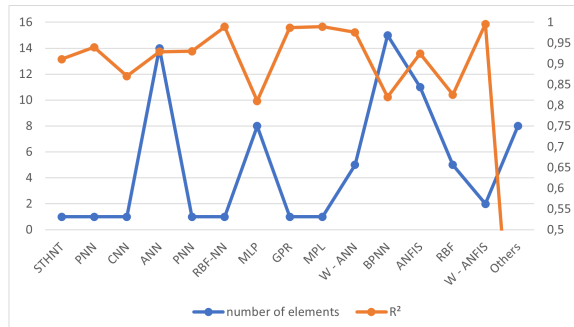

Figure 3: Frequency and accuracy of application of neural networks in WQA

Unlike the paper (Ighalo, Adeniyi, and Gonçalo 2021) we are partially updating, we want to discuss the relationship between the frequency of model usage and their R^2 results. This is to understand whether the reason for model usage is driven by higher accuracy or if there is still a disorganized experimentation with models, without following a systematic approach in this research field. From Figure 3, unfortunately, BPNN models do not yield exceptional results and are among the models with lower performance. On the other hand, ANFIS and ANN show an improvement. These observations indicate that currently there is a lack of order in the experimentation in this field. However, with a critical eye and evaluating each case, ANN and ANFIS are likely the most useful models for data predictions in water quality monitoring.

Conclusion In conclusion, our updated analysis of research on surface water quality assessment using neural network models provides valuable insights and a comprehensive overview of the field. We observed a consistent number of papers published over the past decade, indicating the ongoing development and interest in this area. The most frequently utilized models were BPNN, ANFIS, and ANN, with BPNN emerging as the most popular model in our analysis. However, it is important to note that BPNN did not demonstrate exceptional results compared to other models. Despite the lack of a systematic approach in model experimentation, ANN and ANFIS show promise as useful models for data predictions in water quality monitoring. Further research and development are needed to enhance the accuracy and performance of these models in the field.

Conclusions

In conclusion, the use of AI models in water quality management has a significant social impact. It addresses various concerns such as protecting wildlife, preserving biodiversity, ensuring environmental sustainability, promoting economic prosperity, and improving the well-being of society. By encouraging interdisciplinary research and embracing AI technologies, we are working towards a sustainable future where everyone has access to clean water, ecosystems thrive, and communities prosper.

Our analysis and contributions to this emerging field highlight its potential for further advancements in water quality monitoring with AI. Through ongoing efforts, we can drive positive change and create a healthier and better future for all.

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