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MACHINE LEARNING-BASED FORECASTING OF BIOACCUMULATION AND HISTOPATHOLOGICAL EFFECTS IN AQUATIC ORGANISMS

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ABSTRACT
Heavy metal contamination in freshwater environments poses significant risks to aquatic organisms and human health, as these heavy metals enter freshwater systems through various sources, including industrial waste, agricultural runoff, mining and atmospheric deposition. Efforts to develop efficient methods for removing heavy metals from wastewater have gained momentum in recent years. This study focuses on machine learning (ML) models for predicting the bioaccumulation and histopathological effects of heavy metal pollutants on aquatic life under various climate change scenarios. The ML models have shown promise in forecasting the impacts of heavy metal pollution on freshwater ecosystems and informing conservation strategies. It is crucial to understand the complex interactions between environmental factors, climate change and ecosystem health. This study discusses the importance of incorporating diverse species and environmental factors in these models and acknowledges potential challenges, such as inaccuracies and data misinterpretation. Enhancing the predictive capabilities of ML models is essential for better environmental management and conservation practices via refinement and validation of models using updated data and advanced methodologies. This study also emphasizes the broad potential of ML in environmental research, improvement of model capabilities and challenges posed by heavy metal pollution and climate change.

Keywords: Heavy metal, Contamination, Machine learning (ML) models, Bioaccumulation, Histopathological effects

INTRODUCTION
Heavy metal contamination in freshwater environments presents substantial risks to both aquatic organisms and human well-being as depicted in Figure 1. Among many pollutants, metals are the most dangerous because they can be accumulated and magnified, they are persistent and it is widespread in the water table, sediment and the living organisms that live in these ecosystems (Obadimu *et al*., 2024; Petrea *et al*., 2020; Yaseen, 2021). Several metals, including Iron (Fe), zinc (Zn), copper (Cu), cobalt (Co), manganese (Mn), nickel (Ni), chromium (Cr) and selenium (S) are among the elements that are important for the vital metabolic processes of freshwater ecosystems (Camacho *et al*., 2020; Petrea *et al*., 2020; S. E. Shaibu *et al*., 2024, Ubong *et al*., 2023a and 2023b). Conversely, non-essential metals like lead (Pb) and cadmium (Cd) are useless to the biological processes occurring inside these ecosystems. When present in excess, both necessary and non-essential elements-such as heavy metals-may be hazardous (Bibi, 2023). The accumulation of these heavy metals in freshwater ecosystems is further influenced by the presence of alkali metals, such as sodium (Na) and potassium (K), as well as alkaline earth metals, such as calcium (Ca) and magnesium (Mg) (Camacho *et al*., 2020). However, these heavy metals infiltrate freshwater systems through various routes, such as industrial waste, agricultural runoff, mining and atmospheric deposition (Ciszewski & Grygar, 2016; Vardhan *et al*., 2019). Upon entering the aquatic environment, these heavy metals experience complex chemical and biological changes, impacting their bioavailability, toxicity and persistence (Edo *et al*., 2024). Exposure to heavy metals can result in numerous detrimental effects on aquatic life, including behavioral changes, decreased growth and reproduction and heightened mortality. Additionally, heavy metals can accumulate in aquatic organisms, leading to potential biomagnification throughout the food chain and posing risks to higher trophic levels, including humans (Parida & Patel, 2023).

Given the exacerbating effects of climate change, it is crucial to develop advanced methods for predicting the bioaccumulation and histopathological effects of heavy metals on aquatic organisms (Abiona *et al*., 2019; Khan *et al*., 2018). Traditional laboratory analysis of heavy metal concentrations can be inefficient due to constraints such as resource limitations, staff shortages, high costs of field monitoring and safety issues that can delay results and hinder timely response to pollution events. To overcome these challenges, prediction methods have been proposed to reduce monitoring costs and provide early warnings during heavy metal pollution occurrences. This highlights the need for sophisticated, computer-aided technologies to address these issues (Abiona *et al*., 2019; Jin *et al*., 2020; Liu *et al*., 2018; Zamora-Ledezma *et al*., 2021). Machine learning is essential for addressing the complexities of predicting heavy metal bioaccumulation and histopathological effects in aquatic organisms. ML can efficiently process vast datasets, identify patterns, and provide accurate forecasts, enabling timely, cost-effective decision-making for environmental monitoring and pollution management (Bashir *et al*., 2016).

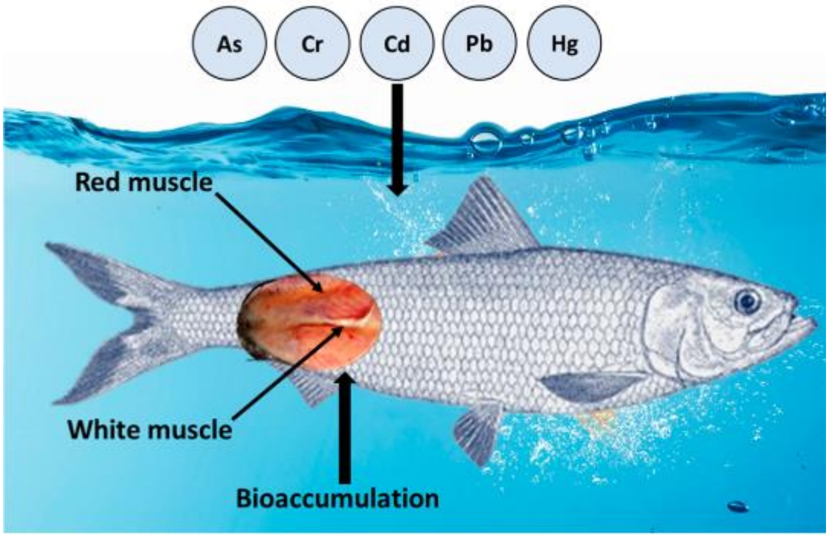

Figure 1: Heavy metal bioaccumulation and metalloid toxicity in fish muscle tissues (Simionov *et al*., 2021)

Recently, machine learning (ML) based heavy metal simulation has gained traction as a potential solution to address the challenges of monitoring and predicting heavy metal pollution. Although various ML algorithms can be employed, the overall workflow required to deploy a comprehensive predictive technological solution remains consistent, as depicted in Figure 2. ML, a subset of artificial intelligence, specializes in identifying patterns within data autonomously as shown in Figure 3. ML-based models employ experimental and automatic learning processes, eliminating the need for explicit programming (Bashir *et al*., 2016; Elsebakhi *et al*., 2015). In essence, the learning model acquires knowledge from samples rather than adhering to strict rules or limited hypotheses. The application of ML can enhance computational efficiency and reliability while reducing associated costs. Moreover, it enables the generation of accurate models through rapid data analysis. With the ability to process vast amounts of data that surpass human comprehension, machine learning equips us with powerful tools for managing large datasets (Mahesh, 2020; Rahmani *et al*., 2021, 2021). By harnessing intricate environmental data and simulating potential outcomes, ML can guide targeted mitigation strategies and inform regulatory policies for preserving freshwater ecosystems. The integration of data-driven insights with conventional environmental monitoring and risk assessment techniques will strengthen our capacity to predict and mitigate heavy metal pollution, ultimately safeguarding the health of freshwater ecosystems and the well-being of the communities that depend on them (Bhagat *et al*., 2022; Yaseen, 2021). This review aims to harness the potential of ML to better understand and predict heavy metal accumulation and its impacts on aquatic organisms under various climate change scenarios. By analyzing complex environmental data and simulating potential outcomes, ML can help guide targeted mitigation strategies and inform regulatory policies for preserving freshwater ecosystems.

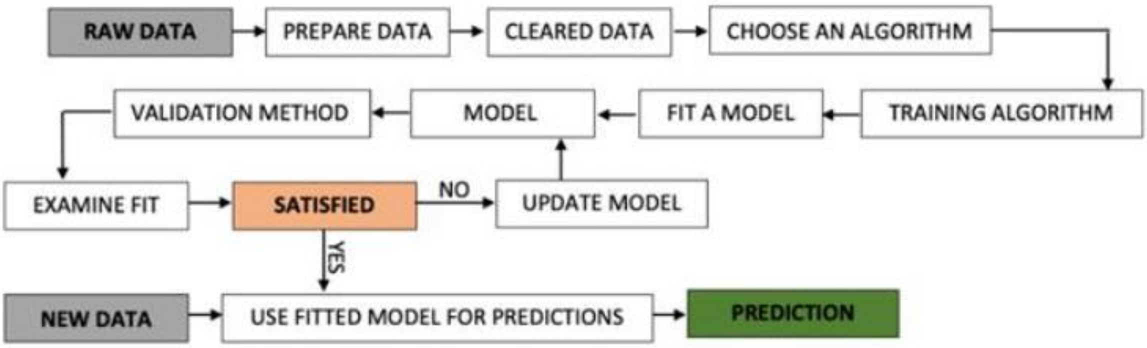

Figure 2: Typical workflow for machine learning (Petrea *et al*., 2020)

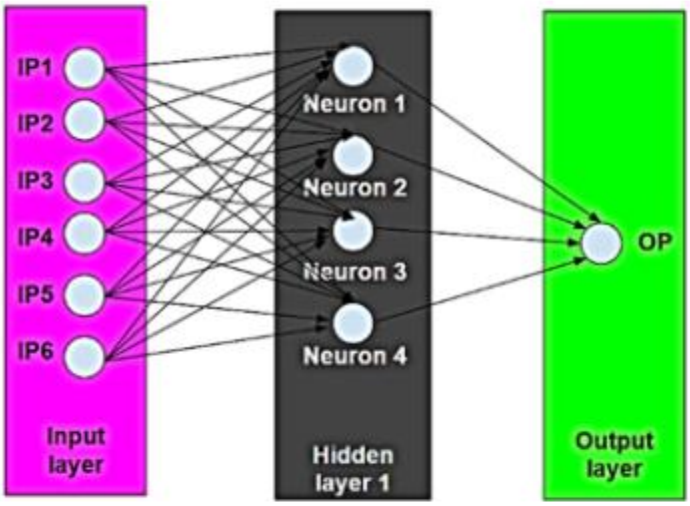

Figure 3: A sample of the architecture of an artificial neural network (ANN) (Hafsa *et al*., 2020)

The purpose of this study is to give insight to the applications of machine learning-based forecasting models to predict the bioaccumulation and histopathological effects of heavy metals in aquatic organisms, providing an efficient and cost-effective alternative to traditional monitoring methods for early detection and management of heavy metal pollution in freshwater ecosystems.

Heavy Metal Pollutants and Their Effects

The environment encompasses the surroundings in which humans, plants, animals and microorganisms exist or function. It consists of land, Earth's atmosphere and water, with the Earth's system defined by four interconnected spheres: the biosphere (living organisms), atmosphere (air), lithosphere (land) and hydrosphere (water), as illustrated in Figure 4. These spheres collaborate and interact harmoniously, contributing to the overall functioning of the Earth's system (Briffa *et al*., 2020). Because of an increase in anthropogenic and geological activity, heavy metal contamination-related environmental challenges are becoming more problematic in emerging nations. These activities raise these elements' concentrations to levels that are detrimental to the environment (Fu & Xi, 2020). The trend of fast industrialization and urbanization has led to an increase in traffic activity, which in turn has contributed significantly to the build-up of heavy metals released into the environment by automobiles. Due to traffic emissions, heavy metal pollution in agricultural areas has the potential to damage crops growing in the surrounding soil (Amoatey & Baawain, 2019). According to Timothy & Tagui Williams (2019), heavy metals, such as copper, lead and zinc, are common transition metals with a density greater than 5 g/cm³ and a relative atomic mass above 40. Fifty-three of the ninety naturally occurring elements fall under this category. Heavy metals have a specific gravity four to five times higher than water under identical temperature and pressure conditions. Additionally, metal elements possess positive valences and are found in groups I to III of the periodic table. Long-term exposure to heavy metals has been associated with neurological disorders, developmental issues and various other health problems. Therefore, comprehending and mitigating heavy metal pollution is crucial for protecting aquatic ecosystems. The bioaccumulation of metals in organisms can lead to various histopathological effects, including cellular damage, oxidative stress, organ dysfunction, immune system impairment and reproductive and developmental issues (Korotkov, 2023; Kumar *et al*., 2024). However, Korotkov, (2023), asserts that heavy metals can cause direct cellular damage by affecting crucial cellular structures like membranes, mitochondria and nuclei, leading to impaired cell function and consequent tissue and organ damage. Moreover, heavy metals stimulate the production of reactive oxygen species (ROS), resulting in oxidative stress, inflammation and DNA damage within cells, a finding supported by numerous other researchers in the field (Goyal *et al*., 2020; Kiran *et al*., 2022; Sun *et al*., 2022). Similarly, Derouiche *et al*., (2020) confirmed that chronic exposure to heavy metals results in the dysfunction of vital organs such as the liver, kidneys and brain, compromising overall organism health. Furthermore, heavy metal toxicity negatively impacts the immune system, increasing susceptibility to infections and diseases. The accumulation of heavy metals in organisms can result in reproductive and developmental issues, leading to abnormalities that negatively impact population growth and long-term ecosystem health. It is crucial to prioritize the development of effective methods for predicting and mitigating heavy metal pollution to protect aquatic ecosystems and ensure the well-being of communities that depend on these resources. The increasing heavy metal concentrations displayed in Figure 5 emphasize the urgency of addressing the issue, as they result from escalating anthropogenic activities that introduce these pollutants into the environment.

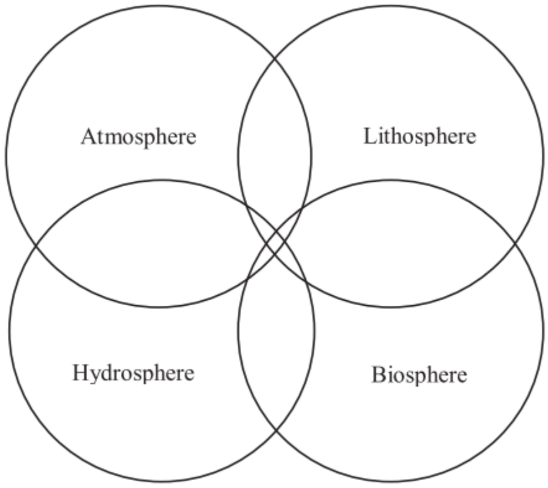

Figure 4: Relationships between each sphere (Briffa *et al*., 2020)

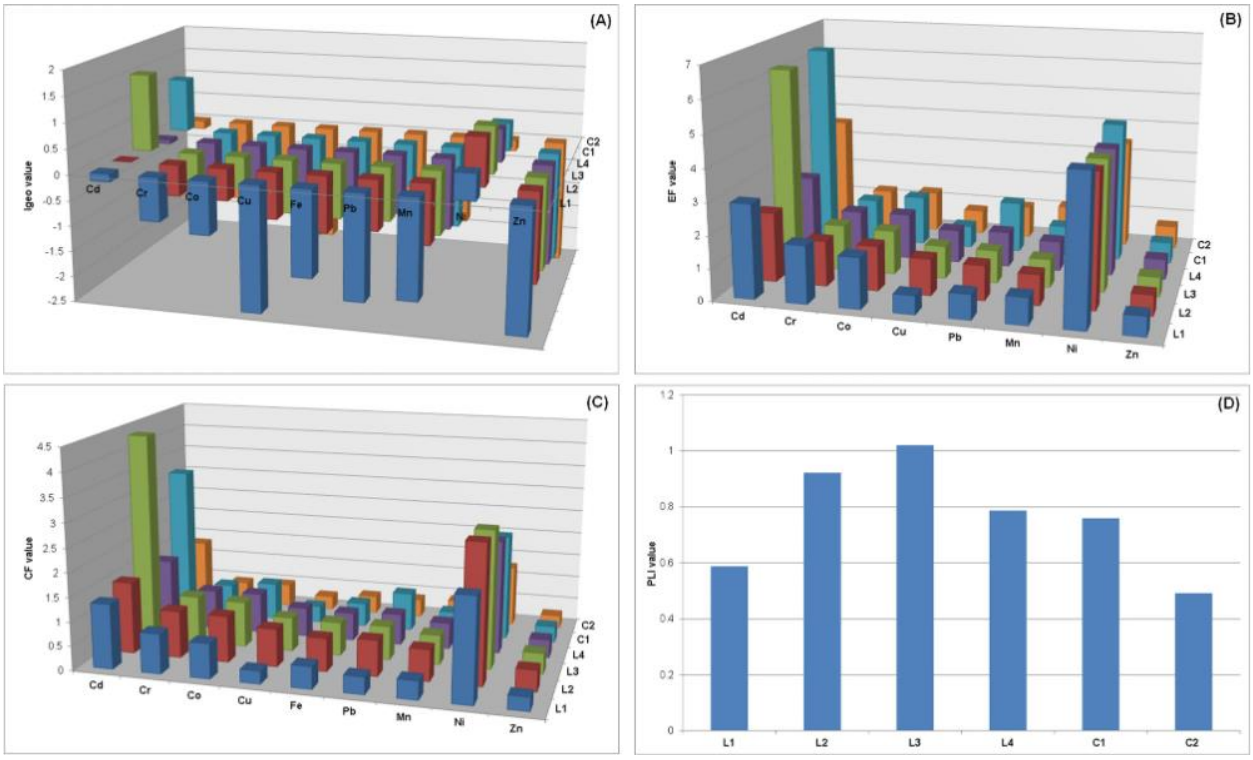

Figure 5: For the shallow sediment of Lake Bafa, the following are shown: (A) heavy metal geoaccumulation indices (Igeos); (B) enrichment factors (EFs); (C) contamination factors (CFs); and (D) pollution load indices (PLIs) (Algül & Beyhan, 2020)

Machine Learning Approaches for Predicting Heavy Metal Bioaccumulation and Histopathological Effects

Overview of Machine Learning Algorithms and Techniques in Aquatic Ecosystems

Machine learning (ML) approaches involve a diverse set of algorithms and techniques, ranging from evolutionary algorithms, solution trees and artificial neural networks to statistical methods, Bayesian networks and metric approaches such as Support Vector Classification and K-Nearest-Neighbor (Mnyawami *et al*., 2022). However, ML approaches are used to create models that can predict outcomes based on data. ML models can be used to solve problems in a variety of fields, from healthcare to finance and can also be used to detect patterns and trends in data, which can help to identify potential risks or opportunities (Eneh *et al*., 2024; Sarker, 2021). These methods aim to address the fundamental issue of anticipating potential outcomes based on current conditions in an aquatic ecosystem, focusing on heavy metal pollutants (Shaibu *et al.*, 2015) and their impacts on aquatic life under climate change scenarios.

ML approaches offer algorithms capable of learning and providing expert-level insights into specific topics. These algorithms are broadly categorized into two major classes based on their learning capabilities which include supervised learning and unsupervised learning (Alloghani *et al*., 2020). The machine learning domain is thriving, particularly with the rise of deep learning as its leading methodology, according to Pouyanfar *et al*., (2019). Deep learning utilizes multiple layers to create computational models that effectively represent data abstractions. Key deep learning algorithms, such as generative adversarial networks, convolutional neural networks and model transfers, have revolutionized information processing.

Moreover, despite rapid advancements in deep learning, a gap in understanding remains due to the lack of a multiscope perspective. This limitation impedes fundamental development by rendering deep learning techniques as black-box machines that are difficult to comprehend and optimize. Furthermore, reinforcement learning algorithms have been identified as another critical category within machine learning, as mentioned by Li, (2017). Supervised learning aims to map inputs to outputs, where input data represents specific instances or examples of interest and outputs correspond to the results provided by a supervisor. Supervised learning tasks are further divided into classification and regression tasks. In classification, output labels are discrete, while they are continuous in regression (Alzubi *et al*., 2018). As a type of supervised learning, classification utilizes a discriminant function to divide examples into distinct classes (Muhamedyev, 2015). By distinguishing finite object groups from a potentially infinite set, supervised learning solves classification problems. Machine learning algorithms within supervised learning include decision trees, support vector machines, regression analysis and Naive Bayes.

To address the challenges of predicting heavy metal bioaccumulation and histopathological effects in freshwater ecosystems under climate change scenarios, ML algorithms can be employed to analyze existing data and discover complex patterns. This enables more accurate predictions of heavy metal concentrations and their associated impacts on aquatic life. Both supervised and unsupervised learning techniques can be utilized to explore and model these intricate relationships, ultimately contributing to better-informed strategies for ecosystem management and mitigation of heavy metal pollution under climate change. However, as shown in Table 1, a comprehensive overview of the various machine learning algorithms and techniques applicable to aquatic ecosystems, along with their descriptions and potential applications in the context of heavy metal pollution has been provided. These algorithms and techniques have potential, but there are still several issues that need to be resolved. These include the lack of high-quality data, the requirement for increasingly sophisticated computing resources and the creation of interfaces that are easy to use for decision-makers and environmental researchers. Researchers can gain a better understanding of heavy metal bioaccumulation and the histopathological impacts on aquatic life under climate change scenarios by overcoming these obstacles and effectively utilizing the potential of machine learning.

Table 1: Overview of Machine Learning Algorithms and Techniques in Aquatic Ecosystems

Algorithm/Technique	Description	Application in Aquatic Ecosystems
Supervised Learning	Uses labeled data to train models for predicting outcomes	Predicting heavy metal concentrations, bioaccumulation and histopathological effects
Decision Trees	Tree-like models for classification and regression	Understanding relationships between environmental factors and heavy metal concentrations
Support Vector Machines	Separates data points into distinct classes using hyperplanes	Predicting impacts of heavy metal pollution on aquatic life
Regression Analysis	Investigates the relationship between dependent and independent variables	Estimating heavy metal concentrations based on environmental conditions
Naive Bayes	Probabilistic classifier based on Bayes' theorem	Assessing risks associated with heavy metal pollution in aquatic ecosystems
Unsupervised Learning	Discovers patterns in unlabeled data	Identifying hidden patterns and trends in aquatic ecosystems
Clustering	Groups data points based on similar characteristics	Organizing data on heavy metal concentrations and impacts
Association Rule Discovery	Identifies relationships between variables	Detecting connections between heavy metals and their sources in aquatic environments
Deep Learning	Utilizes multiple layers to model complex patterns in data	Advanced prediction of heavy metal pollution under climate change scenarios
Convolutional Neural Networks	Analyzes grid-like structured data, such as images	Processing satellite imagery for monitoring aquatic ecosystems
Generative Adversarial Networks	Generates realistic data samples from a given dataset	Simulating potential heavy metal pollution scenarios
Reinforcement Learning	Learns from interactions with the environment to maximize rewards	Optimizing management strategies for mitigating heavy metal pollution in aquatic ecosystems

Data collection and preprocessing for machine learning models

The efficacy of machine learning models is highly dependent on the completeness and caliber of the data used for both training and validation (Arathy Nair *et al*., 2024). Data collection for example includes gathering thorough information about water quality metrics, heavy metal concentrations and biological indicators from freshwater ecosystems. There are three main approaches to data collecting. Firstly, to exchange and search fresh datasets, data collection techniques can be employed for discovery, augmentation, or generation (Huber *et al*., 2021). Once the datasets are accessible, several labeling techniques can be utilized to identify specific cases. In addition, instead of labeling fresh datasets, consider improving existing data or training on previously taught models (Roh *et al*., 2021). Data preprocessing is a useful tool that allows users to treat and analyze complex data; yet, it may consume a significant amount of processing time. It encompasses several different fields, including methods for data reduction and preparation. While the latter aims to reduce the complexity of the data through feature selection, instance selection, or discretization, the former entails data translation, integration, cleansing and normalization (García *et al*., 2016). A dependable and appropriate source for any future data mining technique can be the final data set acquired after a successful data preprocessing stage.

Feature Selection and Engineering for Predictive Models

In the context of predicting heavy metal bioaccumulation and histopathological effects on aquatic life under climate change scenarios, feature selection and engineering are crucial steps in building effective machine-learning models according to Alabdulwahab & Moon, (2020). These processes involve choosing the most relevant features and creating additional useful features to improve model performance (Uddin *et al*., 2018). Feature selection is a dimensionality reduction strategy that aims to choose a small subset of significant features from the original list by eliminating superfluous, redundant, or noisy features (Li *et al*., 2018; Theng & Bhoyar, 2024). This leads to enhanced learning performance, reduced computational costs and more interpretable models. It ensures that the model is trained on the most relevant and impactful data points, resulting in more accurate predictions of heavy metal concentrations and their associated impacts on aquatic life. Conversely, feature engineering is the act of generating new features from preexisting data to enhance model performance, according to Li *et al*., (2017). Discovering temporal and spatial trends may entail crafting interaction terms, constructing polynomial characteristics, or combining data across time and place. For the training, validation and testing stages, methods like data cleaning and resampling optimize the data (Jia *et al*., 2021). For example, combining data on water pH, temperature and metal concentrations can result in a more informative feature that better predicts the bioaccumulation of heavy metals in aquatic organisms. However, optimizing hyperparameters is essential before training the model, as they significantly impact model performance but cannot be learned by the algorithm itself (Jia *et al*., 2021). Similarly, Tripathi *et al*., (2021) confirmed that by carefully selecting and engineering features, researchers can build more robust models that accurately predict heavy metal pollution and its effects on aquatic ecosystems under climate change scenarios, ultimately contributing to better-informed strategies for ecosystem management and pollution mitigation.

Model Training, Validation and Testing for Predictive Analysis in Aquatic Ecosystems

Developing machine learning models for predicting heavy metal bioaccumulation and histopathological effects on aquatic life under climate change scenarios requires careful attention to model training, validation and testing. These steps are crucial for ensuring accurate and reliable predictions from the models (Kumar *et al*., 2024; Petrea *et al*., 2020; Yaseen, 2021). During model training, a subset of available data is used to teach the model to identify patterns and make predictions (Bergen *et al*., 2019). Cross-validation techniques are often employed during this stage to help the model generalize well to new data and avoid overfitting the training set (Küchler *et al*., 2024; Mao *et al*., 2024). Methods like leave-one-out cross-validation (LOOCV) and triple cross-validation can validate models and evaluate their performance across multiple datasets by repeatedly training the model with different subsets of data for validation and training. Validation is a critical phase for assessing the model's performance and making necessary adjustments. This involves optimizing hyperparameters, such as the learning rates of neural networks or the number of trees in a random forest, to improve the model's accuracy and efficiency (Rodriguez-Galiano *et al*., 2015). Additionally, optimization helps refine the model's predictive capabilities, enabling researchers to determine the most effective modeling strategies for heavy metal pollution and its impacts on freshwater ecosystems under climate change scenarios (Zhu *et al*., 2018). In addition, by thoughtfully executing the model training, validation and testing processes, researchers can develop robust predictive tools that support decision-making and contribute to better management of aquatic ecosystems. These models can aid in targeted interventions and mitigation strategies for heavy metal pollution while also deepening our understanding of the complex relationships between environmental factors, heavy metal bioaccumulation and histopathological effects on aquatic life.

Study area and dataset description

To predict bioaccumulation and histopathological effects under climate change scenarios, a thorough understanding of how environmental changes affect chemical accumulation in organisms and the ensuing health implications is necessary. According to Vieira *et al*., (2022), specimens of fish (omnivorous/herbivorous and carnivorous) collected along the Doce River and its affluent Guandú River, as well as in various lakes and coastal lagoons adjacent to the river channel, in the Espirito Santo State, Southeast of Brazil, were used to study multi-biomarker responses and metals bioaccumulation in the fish community of different trophic levels. Even four years after the rupture, it was found that the release of mineral residues from the Fundão mine dam rupture affects the health status of fish from the Doce River basin, causing metals to bioaccumulate, hepatic and brachial damage and increased enzyme activity linked to metal contamination (Umoren *et al*., 2024). The impacts of dam rupture are still felt today in several regions of the world with a long-term effect on the aquatic ecosystems in the region. The long-term health of fish populations in this region remains a concern, as the effects of the dam rupture continue to persist (Ge *et al*., 2020; Pokhrel *et al*., 2018). For instance, in Nigeria, similar concerns about the long-term effects of dam ruptures on aquatic ecosystems have been raised (Bello *et al*., 2024). The potential impacts of dam failures on fish populations in Nigeria, particularly in the Niger Delta region, are a significant concern due to extensive oil and gas exploration activities leading to environmental degradation (Moses *et al.*, 2022). As illustrated in Figure 6, these activities result in heavy metal bioaccumulation, which poses a risk to fish populations and the overall health of the aquatic ecosystem. The Niger Delta serves as a critical example of the potential consequences of industrial activities on local fish populations, underscoring the need for effective environmental management practices to mitigate these impacts.

Figure 6: Extensive oil and gas exploration activities leading to environmental degradation (Shaibu *et al*., 2023)

Furthermore, the Great Lakes, the polar areas and other delicate ecosystems that function as markers of more significant ecological shifts are notable examples (Watson *et al*., 2018). For example, scientists have studied species like the mottled sculpin, lake trout and round goby in the Great Lakes (Robinson *et al*., 2021). These species are essential to the ecosystem and are vulnerable to changes in the temperature as well as chemical exposure. These prediction studies make use of diverse datasets that cover a range of biological and environmental factors. Metrics that can affect both chemical dynamics and biological reactions, such as temperature, precipitation and other climatic factors, are commonly included in environmental data. Furthermore, chemical concentration measurements are essential because they reveal the concentrations of contaminants in sediment, water and living things. Understanding how various chemicals build up over time and their possible health impacts is made possible by this information (Volkel *et al*., 2021). By integrating environmental, biological and historical data from case study sites, the machine learning approach predicts heavy metal bioaccumulation and histopathological effects on aquatic life under various climate change scenarios as confirmed by several researchers (Petrea *et al*., 2020; Rodriguez-Galiano *et al*., 2015). This comprehensive analysis will provide valuable insights for environmental management practices and policies to safeguard aquatic ecosystems and their inhabitants from the adverse impacts of heavy metal pollution.

Development and Training of Machine Learning Models for Predicting Bioaccumulation and Histopathological Effects under Climate Change

Machine learning approaches can be utilized to predict the bioaccumulation of chemicals in wildlife and the resulting histopathological effects under different climate change scenarios (Abiaobo *et al*., 2020; Bawuro *et al*., 2018). The development of these predictive models involves several key steps. First, it is essential to compile a comprehensive dataset of chemical properties, bioaccumulation factors and histopathological endpoints across various species and climate conditions. This process necessitates integrating data from multiple sources and ensuring the quality of the data. Next, preprocessing the data is crucial. This involves handling missing values, encoding categorical variables and normalizing numerical features. Feature selection techniques can then be employed to identify the most important predictors of bioaccumulation and histopathological effects. Following this, the dataset needs to be split into training, validation and test sets to evaluate model performance. Common machine-learning algorithms used in this context include random forests, gradient boosting and neural networks (Grisoni *et al*., 2018). Hyperparameter tuning is performed on the validation set to optimize model complexity. Subsequently, training the machine learning models on the training set is the next step. Regularization techniques such as L1/L2 regularization or dropout can be used to prevent overfitting. The validation set is used to monitor training progress and select the best-performing model. After training, the final model is evaluated on the held-out test set to estimate its generalization performance. Metrics like R-squared, mean absolute error and root mean squared error are used to quantify predictive accuracy. Feature importance scores and partial dependence plots can provide insights into how chemical properties and climate variables influence the predictions (Dawson *et al*., 2023).

Application of Models to predict Bioaccumulation and histopathological Effects under different climate change scenarios

The application of predictive models to examine bioaccumulation and histopathological effects under different climate change scenarios serves as a crucial tool for understanding the implications of climate change on wildlife, ecosystems and their overall health (Guerrera *et al*., 2021). These models can inform policy decisions and strategies aimed at mitigating the impacts of climate change, particularly for species with limited adaptability or mobility. By simulating the effects of changes in temperature, precipitation and extreme weather events on species survival and growth, these models provide valuable insights into the complex dynamics of ecosystems under climate change (Ummenhofer & Meehl, 2017). Despite their usefulness, it is essential to acknowledge the limitations of these models. They often rely on assumptions that may not be entirely accurate, leading to potential inaccuracies in predictions. Additionally, the complexity of these models can result in challenges with interpretation and potential data misinterpretation (Crawford *et al*., 2024).

Accurate data is crucial for the reliability of these models, as it ensures that the predictions made are based on real-world observations rather than hypothetical scenarios. High-quality data allows for better calibration of the models, making the simulations more reflective of actual conditions. Without accurate data, the risk of generating misleading or erroneous results increases, which could lead to ineffective or even harmful policy decisions. Methods for collecting accurate climate data include using satellite observations to monitor temperature, precipitation and other atmospheric conditions on a global scale. Ground-based weather stations provide localized data, offering high-resolution insights into specific regions. Additionally, climate researchers can deploy sensors in oceans, forests and other ecosystems to gather continuous environmental data, which helps to validate and refine predictive models. Once the dataset is prepared, it is utilized to train machine learning models, such as random forests and neural networks (Dawson *et al*., 2023; Rodriguez-Galiano *et al*., 2015). These models are designed to discover correlations between chemical attributes, climatic variables and the resulting histopathological or bioaccumulation endpoints. Hyperparameter tuning is employed to optimize model performance, ensuring that the algorithms can effectively capture complex relationships within the data.

Furthermore, model performance is rigorously evaluated using held-out test sets. Metrics such as R-squared and mean absolute error (MAE) are utilized to assess accuracy, while sensitivity analyses examine how model outputs change in response to variations in input characteristics (Chicco *et al*., 2021). Cross-validation techniques are applied to evaluate the models' ability to generalize to new, unseen data, enhancing the robustness of the predictions. After confirming strong model performance, the trained models are deployed to forecast bioaccumulation and histopathological impacts of chemicals under various climate change scenarios, such as RCP 2.6 versus RCP 8.5. This phase enables researchers to predict how animal bioaccumulation patterns and the fate of chemicals will evolve in response to changing climatic conditions (Anand *et al*., 2020; Kothiyal *et al*., 2023). To validate these predictions, it is crucial to measure bias and accuracy by comparing model outputs to empirical data. Additionally, data uncertainty is incorporated into model predictions through Monte Carlo simulations, which help quantify the potential variability and reliability of the forecasts (Hassan *et al*., 2009; Maia *et al*., 2024).

CONCLUSION

Environmental protection is particularly concerned about heavy metal pollution in aquatic ecosystems. This work effectively demonstrated how machine learning models may be used to forecast the bioaccumulation and histopathological consequences of heavy metal pollution on aquatic life in a variety of climate change scenarios. The results underline how important it is to understand how environmental variables, climate change and the general health of freshwater ecosystems interact. The models that have been built show promise in predicting the effects of heavy metal pollution on aquatic species, providing important data for conservation and policy decisions. It is imperative, therefore, to recognize the limits of these models, including potential errors and misinterpreted data. Although machine learning has a wide range of potential applications in environmental research, future studies should concentrate on refining and validating these models using updated data and advanced methodologies. This will improve their predictive capabilities and contribute to a more holistic understanding of heavy metal pollutants' effects on aquatic ecosystems under climate change scenarios. By incorporating a broader spectrum of species and environmental factors, researchers can enhance the comprehensiveness and applicability of these models for environmental management and conservation purposes.

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