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Heavy metal risk assessment in coastal and inland waters and sediments: A critical review of analytical evolution, ecosystem-based monitoring, and machine learning approaches

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ABSTRACT

Heavy metal contamination in coastal and inland water ecosystems remains a persistent environmental challenge because sediments act not only as long-term sinks of toxic elements but also as potential secondary sources under changing physicochemical conditions. This review examines the methodological evolution of heavy metal assessment from classical wet-chemical and spectrophotometric approaches to modern spectrometric techniques and, more recently, to data-driven machine learning applications for sediment risk prediction. Particular emphasis is placed on the complementary roles of sediment and water sampling within an ecosystem-based monitoring framework, the analytical strengths and limitations of key techniques including atomic absorption spectrometry (AAS), inductively coupled plasma optical emission spectrometry (ICP-OES), inductively coupled plasma mass spectrometry (ICP-MS), and X-ray fluorescence (XRF), and the growing use of machine learning algorithms such as Random Forest, artificial neural networks, support vector machines, and boosting models for hotspot identification, ecological risk interpretation, and decision support. The review argues that contemporary sediment quality assessment should move beyond concentration reporting and instead integrate sampling design, matrix-specific analytical constraints, environmental context, ecological risk indices and predictive modeling within a coherent framework. It further highlights that the scientific and practical value of machine learning depends on representative sampling, robust analytical measurements, transparent preprocessing, appropriate validation strategies, and interpretable modeling approaches. By bringing together analytical chemistry, ecosystem monitoring and artificial intelligence perspectives, this study synthesizes current knowledge, identifies methodological limitations and outlines future priorities for improving heavy metal risk assessment and management in coastal and inland water sediments.

Keywords: Heavy metal risk assessment, Sediment quality assessment, Coastal and inland waters, Ecosystem-based monitoring, AAS, ICP-OES, ICP-MS, Machine learning

Introduction

Coastal and inland water ecosystems are among the most critical environmental systems on Earth in terms of biodiversity conservation, water quality maintenance, food web continuity, and the provision of ecosystem services. Coastal zones, estuaries, deltas, lakes, and rivers are fundamental components of natural systems due to their high ecological productivity and habitat diversity, but they are also subject to intense anthropogenic pressures such as urbanization, industrialization, agricultural drainage, transportation, and port activities (Işık et al., 2025). These pressures lead to increased pollutant loads in aquatic environments, deterioration of water quality, and weakening of ecological integrity. Current studies show that declining water quality, especially in coastal areas, directly affects benthic communities, fish communities, and ecosystem functions, and that in inland waters, ecological integrity should now be evaluated not only with physicochemical criteria but also with biotic structure and ecosystem services (Gotama et al., 2024; Wang, 2024).

In these systems, sediment is not merely a passive reservoir of deposited material but a dynamic environmental archive that records both geogenic background and anthropogenic inputs at the basin scale. Heavy metals and trace elements often accumulate in sediment by binding to suspended solids, fine-grained fractions, Fe-Mn oxides, and organic matter, and therefore sediment is considered a more integrated and persistent indicator of pollution compared to the water column. Global reviews of coastal wetlands and assessments of river sediments reveal that heavy metal pollution is widespread across very different geographies, and sediment is a key medium for monitoring this pressure (Li et al., 2022; Debnath et al., 2021). Furthermore, sediment geochemical properties play a decisive role in the retention, mobility, and bioavailability of metals. Variables such as pH, redox conditions, grain size, organic carbon, and mineralogical composition directly shape metal behavior (Zhang et al., 2014; Miranda et al., 2021).

The environmental significance of heavy metals accumulating in sediment does not stem solely from their total concentration levels. The crucial point is that, under suitable environmental conditions, these elements can re-dissolve into pore water and the overlying water column, thus creating exposure for benthic organisms and generating a wider ecological risk area through trophic transport. In this sense, sediment can function both as a pollutant sink and as a secondary source of pollutants when environmental conditions change. Adsorption-desorption processes, hydrodynamic resuspension, and chemical changes at the sediment-water interface, in particular, cause the risk of heavy metals to vary temporally and spatially (Miranda et al., 2021). Therefore, assessing sediment quality requires a process-based approach that goes beyond simply indicating the presence of pollution; it also aims to understand ecosystem health and risk dynamics.

The analytical methods used to determine heavy metals and trace elements have also undergone a significant transformation in parallel with the development of this research field. While early environmental studies primarily utilized wet chemistry-based separation and colorimetric techniques, the widespread adoption of atomic absorption spectrometry (AAS) marked a significant turning point in trace metal analysis. AAS was used for many years as a fundamental method, particularly due to its reliable and relatively economical metal determination in environmental samples (Beck, 2000). Later, graphite furnace systems lowered detection limits; subsequently, from the 1970s onwards, ICP-OES, with its multi-element, rapid, and sensitive analytical capabilities, gained a strong foothold in environmental monitoring studies. The commercial widespread adoption of ICP-OES from 1974 onwards created a significant technical leap in trace and ultra-trace element analysis (Douvris & Zachariadis, 2023). In the period that followed, ICP-MS, thanks to its much lower detection limits and high sensitivity, became one of the main methods for trace/ultra-trace metal analysis in water, sediment, and soil. Hybrid techniques such as LC-ICP-MS have enabled element speciation studies, contributing to a more detailed assessment of environmental processes (Tiwari et al., 2025). In recent years, field-based techniques such as portable XRF have offered rapid, on-site, and relatively low-cost preliminary assessments, while increasing the flexibility of environmental monitoring programs when used in conjunction with laboratory-based methods (Caporale & Adamo, 2018).

Traditionally, sediment quality guidelines and various geochemical indices are used to interpret heavy metal pollution in sediments. In particular, effects range-low/effects range-median (ERL/ERM) values in marine and estuarine systems, and threshold effect level/probable effect level (TEL/PEL) values and consensus-based quality guidelines in freshwater systems, help to interpret the potential effects of sediment-borne pollutants on benthic organisms at a preliminary assessment level (Long et al., 1995; MacDonald et al., 2000). Current literature reveals that direct and universal interpretation of sediment metal indices is not always appropriate. It is emphasized that assessments made without considering background geochemistry, grain size characteristics, mineralogical variations, and local environmental conditions can lead to

misleading and context-detached results (Birch, 2023). Therefore, the contemporary approach necessitates that sediment quality be considered not with a singular threshold-overshoot logic, but in conjunction with multiple indices, spatial patterns, environmental context, and process analysis.

This need has significantly increased interest in artificial intelligence, and especially machine learning-based approaches, in recent years. Machine learning is increasingly used in heavy metal research due to its capacity to model nonlinear relationships, analyze complex interactions between numerous environmental variables, predict spatial patterns, and reveal risk drivers more systematically. Interpretable machine learning approaches and explainability tools such as SHapley Additive exPlanations (SHAP) offer significant advantages for environmental decision support processes, as they not only generate predictions but also demonstrate the importance and direction of the variables shaping these predictions. Recent studies show that interpretable machine learning models can yield useful results in ecological risk prediction even under conditions of data scarcity, and that SHAP-based analyses reveal the underlying factors driving pollution more clearly (Chen et al., 2026; Wang et al., 2025).

In this context, water- and sediment-based assessment of heavy metal pollution is no longer limited to classical analytical measurements and index calculations. Current research increasingly considers sampling strategies, analytical determination techniques, sediment-water interactions, guideline-based risk approaches, and data-driven modeling tools within a more holistic assessment framework. The contribution of this review is to integrate the historical development of heavy metal analysis methods with sediment-focused monitoring, ecosystem-based sampling, and machine-learning-supported risk estimation in a single analytical framework. Accordingly, the manuscript does not simply list methods; rather, it discusses how each methodological component strengthens, limits, or complements heavy metal risk assessment in coastal and inland water ecosystems.

Review Methodology and Scope

This study is designed as a structured narrative review that addresses the development of heavy metal analysis methods and the application of machine learning in sediment-based risk assessment. The scope of the review includes studies that evaluate heavy metal determination, sediment and water sampling strategies, ecological risk interpretation, and data-driven prediction approaches in coastal and inland water ecosystems within the same framework. In selecting the literature, priority was given to peer-reviewed publications in the Web of Science, Scopus, ScienceDirect, and Google Scholar databases; current studies from the period 2000-2026 were particularly focused on. However, older but foundational studies were also included to demonstrate the historical development of classical chemical methods, sediment quality guidelines, and analytical transformation.

During the screening process, various combinations of keywords such as "heavy metal analysis," "sediment quality," "water-sediment interaction," "sampling strategy," "ecological risk," "AAS," "ICP-OES," "ICP-MS," "XRF," "machine learning," "interpretable artificial intelligence," "coastal sediment," and "inland water sediment" were considered. Studies were selected not only based on analytical performance but also on the suitability of the methods for the environmental matrix, the context of risk assessment, and their decision support potential. The review included original research, review articles, and authoritative reports that directly contribute to the fields of heavy metal analysis, sediment quality assessment, water-sediment interaction, modern spectrometric techniques, environmental risk indices, and machine learning-based modeling. Publications weakly related to the topic, studies focusing solely on a single parameter without establishing a context for sediment or risk assessment, and records that could not be bibliographically verified were excluded. Therefore, this study is less of a quantitative meta-analysis and more of a transparent and thematic review aiming to explain methodological evolution, trends in the literature, and research gaps.

To respond to the need for a more critical synthesis, the selected literature was evaluated according to five comparative dimensions: matrix compatibility, analytical sensitivity, sample-preparation requirements, suitability for ecological risk interpretation, and capacity to support predictive or decision-oriented assessment. This structure allowed the review to identify not only methodological advantages but also recurrent limitations, including matrix interference, insufficient quality assurance reporting, inconsistent sampling designs, limited open data availability, and weak validation of predictive models.

Evolution of Heavy Metal Analysis Methods

Classical Chemical Methods

In heavy metal analysis, classical chemical methods were among the primary approaches used in the examination of environmental samples, especially during the period from the 1950s to the 1970s. The basic methods used during this period were gravimetric and titrimetric analyses, based on the precipitation, complex formation, or redox transformation of metal ions through appropriate chemical reactions. These methods offered a reliable measurement framework based on

the principles of accuracy, stoichiometry, and reaction completeness in the early days of analytical chemistry; they gained widespread use, particularly due to their low cost and applicability in environments with basic laboratory infrastructure (Amaral et al., 2024; Chormey et al., 2025).

In gravimetric analyses, metal ions are generally precipitated as sparingly soluble compounds, after which the precipitate is filtered, washed, dried or ignited, and weighed to constant mass. The accuracy of this approach depends on complete precipitation, the purity and stability of the precipitate, control of co-precipitation, suitable pH and temperature conditions, and the production of a consistent weighing form (Alotaibi & Nassif, 2024). The principal advantage of gravimetry is its direct dependence on mass and stoichiometric relationships. Although it is now rarely used as a routine method for trace-level environmental monitoring, it remains relevant for high-purity substances, reference-material validation, and analytical chemistry training (Miura, 2024; National Institute of Standards and Technology [NIST], 2025).

Titrimetric methods have proven functional in the determination of heavy metals, particularly in higher concentration ranges. These methods are based on redox, precipitation, or complexometric reactions; they involve reacting metal ions with a standard solution and determining the endpoint by color change, indicator, or potentiometric monitoring. These methods, particularly used for the individual determination of some metals such as iron, copper, zinc, and manganese, have been preferred for a long time due to their low equipment requirements and relative economics. However, titrimetric analyses are highly dependent on the accurate determination of the endpoint, the removal of interfering ions, and the maintenance of the analyte in the appropriate chemical form. Therefore, their reliability remains limited in complex environmental matrices, especially in multi-metal mixtures and at trace concentrations (Amaral et al., 2024; Chormey et al., 2025).

These classical methods have been used not only in water samples but also in solid environmental matrices such as sediment, soil, mud, and similar materials. However, the important point here is that direct determination of metals in solid samples is not possible. In matrices such as sediment, sample preparation requires drying, homogenization, grinding, and subsequent transfer of metal ions to the solution phase through acidic dissolution, ashing, or extraction processes before analysis. Therefore, while gravimetric and titrimetric methods are applicable to sediment, this process is more laborious, time-consuming, and more susceptible to matrix interference compared to water samples. Current environmental analytical literature emphasizes that sample preparation is a fundamental step in determining the accuracy of the method, especially in sediment and other solid samples, in metal analysis (Vesković et al., 2025; Chormey et al., 2025).

The main limitations of classical chemical methods include low sensitivity, high labor requirements, long analysis time, limited element coverage, and the inability to perform simultaneous multi-element analysis. Especially in environmental monitoring studies, since heavy metals are often found at levels of µg/L or lower, gravimetric and titrimetric methods may be insufficient in these concentration ranges (Alotaibi & Nassif, 2024). Furthermore, in complex matrices such as sediment and seawater, high salinity, organic matter content, co-precipitation, matrix pressure, and the presence of interfering ions can reduce the accuracy of the results. Therefore, instrumental techniques such as AAS, ICP-OES, and ICP-MS have largely replaced classical methods due to their advantages of lower detection limits, higher selectivity, multi-element analysis capability, and faster results (Chormey et al., 2025; Shi et al., 2025).

Nevertheless, classical methods have not completely lost their importance. These methods are still used today in analytical chemistry education, in the analysis of some high-concentration industrial samples, in teaching the logic of reference methods, and in some validation applications. Gravimetric analysis, in particular, still provides a strong theoretical foundation for understanding the calibration and validation logic of instrumental methods. Therefore, classical chemical methods represent not only the initial stage in the historical development of heavy metal analysis; they also form the basis of the quality assurance, reaction control, and sample preparation disciplines of modern environmental analytics (Miura, 2024; Amaral et al., 2024).

Spectrophotometric Period

The spectrophotometric era in the development of heavy metal analysis methods is considered a significant transitional phase offering higher sensitivity and more practical measurement possibilities compared to classical chemical methods (Aktaş & Gençer, 2024). This period has become particularly prominent with the widespread adoption of colorimetric and UV-Vis spectrophotometric methods, which are based on the formation of colored complexes of metal ions with specific organic or inorganic reagents. The basic principle is that a metal ion reacts with a suitable chromogenic reagent to form a colored complex that absorbs light at a specific wavelength, and this absorbance is correlated with concentration within the framework of the Beer–Lambert law. Thus, a faster, less labor-intensive, and more useful analysis option for low-to-

medium concentration ranges has emerged compared to gravimetric and titrimetric methods (Bay, 2022). Current assessments also emphasize that colorimetric and absorbance-based approaches in heavy metal determination represent a significant step in the analytical development process, particularly due to their simplicity, low cost, and field applicability (Si et al., 2024; Shi et al., 2025).

The methods used in the spectrophotometric era have become more directly applicable, especially to water samples. Since metal ions are present in solution in liquid matrices such as stream water, lake water, seawater, wastewater, and drinking water, measurements have been possible in most cases with appropriate pH adjustment, addition of complexing reagents, and, if necessary, the use of masking agents. In contrast, spectrophotometric determination in solid matrices such as sediment, soil, and mud is not performed directly, but rather after the sample is first transferred to the liquid phase through acidic dissolution or extraction processes (Alotaibi & Nassif, 2024). Therefore, spectrophotometric methods have also been used for sediment; however, the key to success in sediment analysis has been more about sample preparation and control of matrix interferences than the instrument itself. This distinction explains why water and sediment studies in environmental heavy metal analysis, although mentioned under the same analytical heading, have different process flows (Si et al., 2024; Shi et al., 2025).

One of the most important advantages of this era is that it offers higher sensitivity and shorter analysis times compared to classical methods. Furthermore, the ability to apply spectrophotometric methods in standard laboratories without the need for expensive and advanced equipment infrastructure has long made them attractive. These approaches, based on the complexation behavior of metal ions, have been used to determine many metals such as lead, cadmium, chromium, arsenic, cobalt, mercury, and copper. The selectivity and detection limits of these methods have been improved over time, particularly with the development of selective ligands, azo dyes, Schiff bases, and nanoparticle-supported chromogenic systems. Recent studies show that colorimetric approaches based on color change continue to exist today in new forms such as portable sensors, smartphone-assisted analysis, and rapid field scanning (Hakim & Bilad, 2024; Shahbaz et al., 2024; Fakayode et al., 2023).

However, the use of spectrophotometric methods in heavy metal analysis also has significant limitations. Firstly, these methods often focus on a single element or a limited number of target analytes, and their capacity for simultaneous multi-element analysis is low. Secondly, special complexing agents, specific pH conditions, and interference-reducing agents are needed to ensure sufficient selectivity for many metal ions. In samples with high ionic strength, such as seawater, as well as in sediment extracts, organic matter and accompanying ions can affect color formation or absorbance measurement, reducing accuracy (Dinç, 2019). Therefore, although spectrophotometric methods have constituted an important step forward in environmental monitoring, they have become insufficient over time for the reliable determination of heavy metals at very low concentrations and have been replaced by more selective and multi-element instrumental techniques such as AAS, ICP-OES, and ICP-MS (Shi et al., 2025; Abdelmonem et al., 2025).

On the other hand, the spectrophotometric era should not be seen as merely a historical phase. Today, this approach has regained importance, particularly in terms of low-cost screening, in-situ analysis, rapid preliminary assessment, and the development of color-based sensor technologies. Modern color-change-based sensors can be considered as current extensions of classical spectrophotometric logic combined with nanomaterials, paper-based platforms, and microfluidic systems. In this respect, the spectrophotometric era is more than just a temporary technical phase in the history of heavy metal analysis; it forms the theoretical basis of today's portable and user-friendly analytical systems (Fakayode et al., 2023; Nadumane et al., 2024).

Modern Spectrometric Techniques

Modern spectrometric techniques for heavy metal analysis have formed the basis of environmental analytical chemistry due to their lower detection limits, higher selectivity, capacity for simultaneous multi-element analysis, and shorter analysis times compared to classical chemical and spectrophotometric methods. This transformation is particularly evident with the widespread adoption of techniques such as atomic absorption spectroscopy (AAS), inductively coupled plasma-optical emission spectrometry (ICP-OES), and inductively coupled plasma-mass spectrometry (ICP-MS). Current reviews show that the modern era in heavy metal and trace element analysis is primarily shaped around atomic and plasma-based spectrometric systems; these techniques largely meet the requirements for accuracy, sensitivity, and multi-element analysis in environmental samples (Chormey et al., 2025; He et al., 2024).

These techniques are applicable not only to liquid samples such as stream water, lake water, seawater, groundwater, and wastewater; they are also widely used in solid or semi-solid environmental matrices such as sediment, soil, mud, biota, and plant tissue. However, there is a significant difference in terms of method application between water samples and solid samples such as sediment. While filtration, acid preservation,

and pre-enrichment, when necessary, may often suffice for water samples, sediment requires a more intensive sample preparation process, including drying, grinding, homogenization, and often microwave-assisted or open-system acid dissolution. Therefore, modern spectrometric techniques are directly "suitable" techniques for sediment as well; however, their success, especially in solid samples, depends on the quality of sample preparation as much as on the equipment (Poljak et al., 2024; Provete et al., 2024).

AAS has been one of the first atomic spectrometric techniques widely used in modern heavy metal analysis. Flame AAS (FAAS) and graphite furnace AAS (GFAAS), in particular, have been standard methods for the individual determination of specific metals for many years. The most important advantages of AAS are its relatively lower instrument cost, good accuracy, selective measurement capacity, and accessibility in many laboratories. However, AAS mostly operates on single elements; that is, it is not suitable for the analysis of many metals simultaneously. Furthermore, it shows more limited sensitivity compared to ICP-MS at ultra-trace level concentrations and in very complex matrices. Nevertheless, current literature shows that AAS retains its importance, especially in routine laboratory analyses, in solid samples such as soil and sediment after acid dissolution, and in the verification of target metals in environmental water samples (He et al., 2024; Poljak et al., 2024).

ICP-OES has marked a significant turning point in modern environmental metal analysis. This technique is capable of performing multi-element simultaneous analysis and offers a wider dynamic range compared to AAS. ICP-OES, which is based on measuring the characteristic emission lines emitted as a result of the excitation of atoms and ions in a plasma source, is widely used, especially in environmental samples in the medium and high concentration ranges. While it provides effective results in water samples directly or after appropriate dilution, it can be reliably applied in solid matrices such as sediment and soil after acidic dissolution. The main advantages of ICP-OES include its ability to determine many elements simultaneously, its high sample capacity, and its relatively robust routine analysis infrastructure. However, it is not as sensitive as ICP-MS at very low concentrations and under some interference conditions (Chormey et al., 2025; Provete et al., 2024).

ICP-MS is currently considered one of the leading techniques providing the highest sensitivity in heavy metal and trace element analysis. In this method, elements ionized in plasma are separated according to their mass/charge ratios and can be reliably measured even at very low concentrations. ICP-MS offers significant advantages, particularly in trace- and ultra-trace-level metal determinations, multi-element environmental screenings, in matrices with low concentrations but high interference potential, such as seawater, and in detailed studies requiring risk assessment. In recent years, combining ICP-MS with pre-enrichment systems such as microextraction, magnetic solid-phase extraction, and flow injection has further enhanced the method's capabilities in environmental water samples. Current sources indicate that ICP-MS has become a fundamental reference technique, particularly in environmental monitoring, sediment and water comparisons, bioaccumulation studies, and multi-pollutant screenings (Chormey et al., 2025; Tiwari et al., 2025).

The modern spectrometric era is not limited to AAS, ICP-OES, and ICP-MS. In recent years, X-ray fluorescence spectrometry (XRF), including portable X-ray fluorescence (pXRF), has gained importance, particularly in solid samples such as soil and sediment, due to its ability to provide rapid, non-destructive analysis or analysis requiring minimal preparation. Portable XRF systems offer advantages in terms of field-based preliminary assessment, contamination screening, and sample selection. However, the detection limits of XRF are not as strong as those of ICP-MS, especially in low-concentration environmental samples and for some light elements; therefore, it is often used in conjunction with ICP-based techniques for detailed quantitative verification. Current comparative studies show that pXRF is strong in terms of speed and field applicability, while AAS and ICP-MS perform better, especially in situations requiring high accuracy and low detection limits (Poljak et al., 2024).

However, modern spectrometric techniques also have some limitations. These methods are not equally accessible in all conditions due to high equipment and operating costs, the need for trained personnel, matrix-related spectral and non-spectral interferences, the need for laboratory infrastructure, and time-consuming sample preparation steps, especially in solid samples such as sediment. Matrix pressure and interference effects, particularly in samples with high salinity such as seawater, and incomplete dissolution, heterogeneity, and contamination risk in sediments can affect the quality of the results. Therefore, the current analytical approach relies not only on equipment selection but also on sampling, preservation, dissolution, quality control, the use of certified reference materials, and appropriate calibration strategies (Chormey et al., 2025; Provete et al., 2024).

In conclusion, modern spectrometric techniques have become the standard approach in the evaluation of environmental matrices such as water and sediment in heavy metal analysis. While AAS maintains its importance as a more economical and target element-focused option, ICP-OES stands out in

multi-element routine analyses, and ICP-MS in trace and ultra-trace level determinations. XRF, on the other hand, plays a complementary role, especially in field surveys and rapid solid sample evaluations. In this context, the modern spectrometric era signifies not only the use of more advanced instruments in environmental heavy metal monitoring studies but also the establishment of a more sensitive, faster, more holistic, and matrix-focused analytical approach (He et al., 2024; Chormey et al., 2025).

Figure 1 illustrates the evolution of heavy metal analytical approaches from classical chemical methods to data-driven analytics, highlighting key transitions and improvements in sensitivity, automation, multi-element capacity, and predictive interpretation.

Table 1 presents a comparative evaluation of sediment, water, and integrated sampling strategies in terms of process representation, sampling equipment, methodological strengths, limitations, and proposed applications.

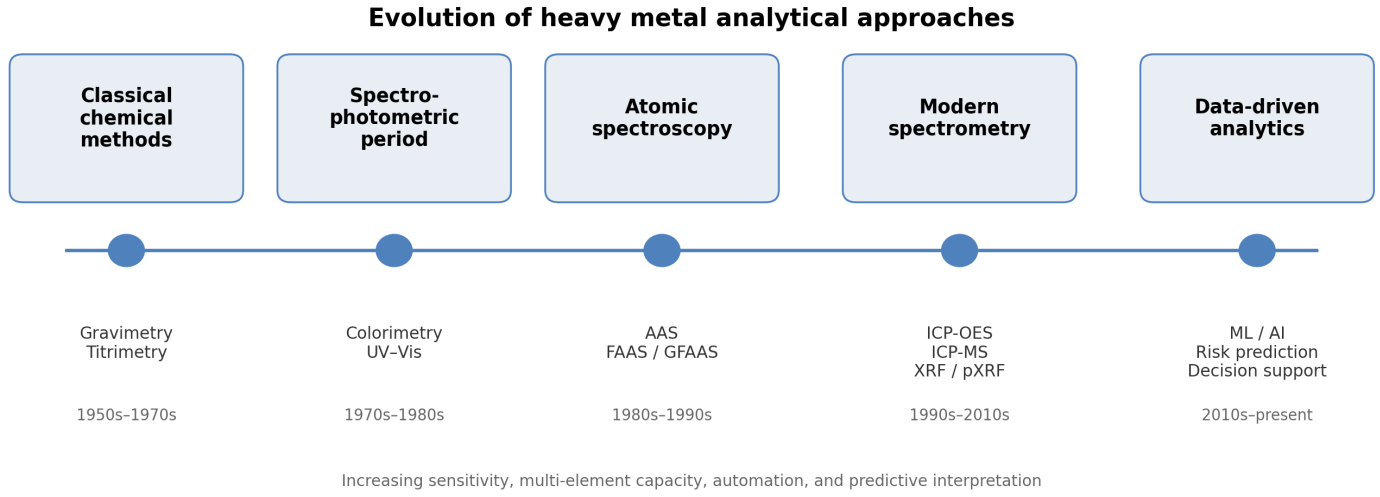

Figure 1. Evolution of heavy metal analytical approaches from classical chemistry to data-driven modeling (created by the authors based on Chormey et al., 2025 and Haque et al., 2025).

Table 1. Comparison of sediment and water sampling strategies

Matrix	Represented process	Main equipment	Main strengths	Main limitations	Recommended use
Sediment	Long-term accumulation and environmental memory	Ekman grab, Van Veen grab, corer/piston samplers	Shows chronic pollution and bottom accumulation	Heterogeneous structure and the need for depth-based sample preparation	Ecological risk indices and historical accumulation analysis
Water	Instantaneous solution and total metal levels	Sampling bottles, Niskin, Van Dorn	Reflects current environmental conditions and active transport	Sensitive to temporary fluctuations and contamination	Monitoring active pollutant inputs and short-term changes
Integrated approach	Joint evaluation of the transport–accumulation relationship	Combined sampling design	Stronger ecosystem interpretation and more reliable risk assessment	Requires more time, cost, and coordination	Recommended as the main strategy for coastal areas and rivers

Sampling Strategies and the Ecosystem-Based Approach

In assessing heavy metal pollution, the sampling strategy is as crucial as the analytical phase because the representativeness of the data obtained largely depends on where, when, at what depth, and with what equipment the sample is taken. In an ecosystem-based approach, the aim is not only to measure pollutant concentration but also to evaluate processes such as metal transport, accumulation, remobilization, and bioavailability within the physical and biochemical functioning of the aquatic system. Therefore, sampling based on a single matrix in river, lake, reservoir, estuary, and coastal marine environments is often considered insufficient; it is recommended to interpret water column, surface sediment, and, if necessary, biota data together (Frincu, 2025). Recent reviews, in particular, emphasize that monitoring heavy metals in aquatic ecosystems in both the dissolved phase and sediment more accurately reveals the sources, persistence, and ecological risk dimensions of pollution (Hossain et al., 2024; El-Sharkawy et al., 2025).

Sediment sampling is of particular importance in environmental assessments because it reflects the long-term accumulation of heavy metals. While metal concentrations in the water column can show significant fluctuations due to short-term hydrological events, flow rate changes, precipitation, tides, suspended solids load, and anthropogenic discharges, sediment often provides a temporally integrated record of these fluctuations (Frincu, 2025). Therefore, sediment data are used as a fundamental data source, especially in the calculation of pollution indicators such as ecological risk index, enrichment factor, geoaccumulation index, and so on. Furthermore, sediment is not only a pollutant reservoir but can also be a secondary source for metals depending on pH, redox potential, grain size distribution, organic matter content, and hydrodynamic conditions; in this respect, it plays a critical role in understanding long-term environmental risk (Hossain et al., 2024; Miranda et al., 2021).

Equipment selection for sediment sampling varies depending on the targeted sediment type and the research question. Grab samplers, such as the Ekman grab and Van Veen grab, are commonly used, especially for collecting surface sediment; they offer practicality in soft-bottomed lakes, river mouths, lagoons, and coastal areas. In contrast, core/piston type samplers are more suitable for studies investigating stratification, historical accumulation, or vertical metal distribution because these systems allow for obtaining chronological information along the depth with less disruption of the sediment profile. Sampling surface sediment with grabs and deep layers with core systems helps to differentiate current contamination from historical accumulation (Frincu, 2025). However, partial disruption of the surface layer, loss of fine fractions, and variability in sample volume are significant sources of uncertainty in grab samplers, while penetration depth, compaction, and difficulty in accessing hard layers are important in core systems. EPA field guidelines also emphasize that equipment selection for sediment sampling should be made in accordance with field conditions and analytical objectives, and that sample degradation and cross-contamination directly affect quality (U.S. Environmental Protection Agency, 2015).

The reliability of sediment data depends not only on the sampler used but also on sampling density, station distribution, depth selection, and the physical heterogeneity of the sediment. Since metal accumulation in streams is often more pronounced in low-flow areas, meanders, behind dams, or in zones dominated by fine-grained sediments, the sampling network should be designed to represent hydrodynamic variations. In lakes and reservoirs, deep basins, inlet-outlet zones, and fine-grained deposition areas are prominent, while in coastal and estuarine systems, tides, salinity gradients, suspended sediment transport, and river inputs determine the sampling design. Because sediment grain size, carbonate and organic matter content, and mineralogical structure directly affect metal retention, not only total metal concentrations but also supporting sedimentological parameters should be measured together whenever possible. This approach is particularly important for distinguishing whether the metal variability observed between different stations may be due not only to pollutant load but also to natural matrix differences (Hossain et al., 2024; U.S. Environmental Protection Agency, 2001).

Water sampling is a fundamental approach that complements sediment data and reveals the instantaneous or short-term chemical status of the system. Dissolved or total metal concentrations are critical, especially in monitoring active pollutant inputs, seasonal variations, and transport processes. While water samples can be taken from the surface using simple bottle sampling, in lakes, reservoirs, estuaries, and marine environments requiring depth profiling, it is possible to take more controlled samples from specific depths using closed-system samplers such as Niskin and Van Dorn. USGS guidelines state that in trace metal sampling, sampler material, transport equipment, and field operations should be selected to minimize contamination; contamination from sampling equipment, especially at low concentration levels, can seriously distort results (Wilde, 1999).

However, water sampling has significant limitations. Dissolved metal levels can often change over short time scales; factors such as precipitation, flooding, industrial discharge,

bottom erosion, salinity changes, and biological activity can cause sudden fluctuations in metal concentrations in the water column. Furthermore, since the concentration of many metals in the dissolved phase is lower than the total load in the sediment, obtaining reliable data becomes difficult without proper containment, filtration, acid stabilization, and clean sampling procedures (Hossain et al., 2024). High ionic strength in seawater and estuary samples, and suspended solids load and heterogeneous flow conditions in river waters, make sample representation difficult. Therefore, while water samples provide a "snapshot" of pollution, sediment samples represent more of its "temporal memory." For a sound interpretation at the ecosystem level, these two pieces of information must be evaluated together (Hossain et al., 2024; Miranda et al., 2021).

In this context, the most appropriate approach in different aquatic ecosystems, such as coastal areas, rivers, and lakes, is an integrated sampling design that plans sediment and water sampling together. In rivers, discharge regime, flow velocity, erosion-deposition balance, and suspended sediment transport should be considered; sampling stations should be selected in a staggered manner along the upstream-pollutant inlet-downstream line. In lakes, thermal stratification, bottom basins, inlet-outlet zones, and benthic accumulation areas; and in coastal and estuarine systems, tidal effects, salinity mixing, sedimentary deposition areas, and river mouths should be the key determinants of design (Hossain et al., 2024). This approach, which combines long-term sediment accumulation information with the instantaneous chemical status of water samples, provides advantages both in the decomposition of pollution sources and in making more realistic ecological risk assessments. Therefore, in ecosystem-based heavy metal monitoring programs, the sampling strategy should be seen not only as a technical field operation but also as a fundamental scientific design stage that integrates the system's operational logic with data (Hossain et al., 2024; El-Sharkawy et al., 2025).

Comparison of Classical and Modern Approaches

The fundamental difference between classical and modern approaches in heavy metal analysis lies not only in the level of equipment used but also in the quantity, accuracy, resolution, and contribution of the generated data to decision support processes. Classical gravimetric, titrimetric, and early spectrophotometric methods have been widely used for many years due to their low equipment cost, applicability in basic laboratory infrastructure, and instructive analytical value. These methods still have a certain function, especially in high-concentration samples, in the determination of a limited number of target metals, and in laboratories lacking advanced instrument infrastructure. However, since current requirements in environmental heavy metal studies often necessitate lower detection limits, multi-element simultaneous analysis, high sample processing capacity, and stronger quality assurance protocols, classical methods often lag behind modern spectrometric techniques (Işık et al., 2025; Shi et al., 2025; Abdelmonem et al., 2025).

The most important advantage of classical approaches is their relatively low cost and accessibility. These methods can be functional, especially in laboratories with limited budgets, for routine training purposes, or for the preliminary evaluation of high-concentration samples. Furthermore, the fact that the analytical logic can be clearly traced through reaction stoichiometry, complex formation, or precipitation chemistry makes these methods valuable in terms of the fundamental principles of analytical chemistry. However, despite these advantages, classical methods are mostly single-element focused, time-consuming, and have high operator dependency. Controlling interference becomes difficult, especially in matrices such as sediment, seawater, and complex wastewater; reliability decreases at low concentration levels; and the analysis time and labor requirements increase significantly in large-scale environmental monitoring studies. Therefore, in today's environmental risk studies, classical methods are often evaluated at the level of preliminary screening or supporting verification rather than detailed characterization (Abdelmonem et al., 2025; Chormey et al., 2025).

This data density has also encouraged the use of machine learning and advanced statistical modeling in environmental heavy metal research. While classical methods often work with a limited number of variables and narrower sample sizes, modern analytical infrastructures generate multidimensional data, thus providing a stronger foundation for classifying pollution sources, identifying spatio-temporal patterns, estimating ecological risk, and modeling future scenarios. Recent reviews and applied studies show that machine learning algorithms are becoming increasingly important in monitoring heavy metal pollution, identifying sources, and increasing the sensitivity of risk assessment. Especially in modern environmental monitoring systems working with large datasets, these approaches enable a shift from purely descriptive analysis to predictive analysis (Haque et al., 2025; Wang et al., 2024; Izah & Ogwu, 2026).

However, the superiority of modern methods does not mean that they are unconditionally the best option in every case. ICP-MS, ICP-OES, or advanced hybrid mass spectrometric techniques may not be sustainable, especially in laboratories

with limited resources, due to high equipment costs, maintenance expenses, consumable consumption, energy requirements, and the need for expert personnel. Furthermore, the increasing volume of data necessitates not only ease of analysis but also a need for data management, quality control, statistical interpretation, and computational infrastructure. Incorrect calibration, inadequate quality assurance practices, or weak data processing strategies can reduce the interpretive value of large datasets obtained with modern techniques. In other words, the use of advanced equipment does not automatically mean better scientific results; these instruments must be supported by appropriate sampling design, correct sample preparation, and a robust statistical framework (Shi et al., 2025; Izah & Ogwu, 2026).

Therefore, the choice of analytical approach in environmental study design should not be based solely on the ranking of technical superiority, but rather on a combined assessment of the research objective, target matrix, expected concentration range, budget, laboratory infrastructure, field conditions, sample size, and required data resolution. While classical or simpler methods may suffice for preliminary investigations, limited-budget monitoring, or evaluation of high-concentration samples, modern spectrometric techniques are significantly more suitable for multi-element, low-concentration, risk-focused, and decision-support studies. Therefore, the most accurate approach is to consider classical and modern methods not as alternatives to each other, but as tools that contribute at different levels depending on the research question. The main goal in current environmental heavy metal research is to move beyond a choice limited by laboratory capabilities and transform the technical selection into a holistic methodological decision compatible with data quality and ecological interpretive power (Abdelmonem et al., 2025; Haque et al., 2025). Table 2 provides a systematic comparison of major heavy metal analysis techniques based on their matrix compatibility, sensitivity, multi-element analysis potential, cost, and key methodological advantages and constraints. Because detection limits and precision ranges vary by element, instrument configuration, digestion protocol, calibration strategy, and matrix composition, the table reports relative sensitivity and the main reporting requirements rather than fixed universal numerical limits.

This comparison also shows that method selection should be reported as a scientific justification rather than as a routine laboratory choice. For example, a study based on ICP-MS is stronger for ultra-trace multi-element screening, but it may still be weak if sediment digestion, certified reference materials, blanks, recovery rates, and matrix effects are not adequately reported. Conversely, simpler methods may provide useful preliminary information when concentration levels are high and when their uncertainty is clearly acknowledged. Therefore, methodological rigor depends on the alignment between research objective, matrix properties, analytical sensitivity, quality assurance, and ecological interpretation.

Table 2. Comparison of heavy metal analysis techniques

Method	Suitable matrix	Sensitivity	Multi-element analysis	Cost	Main advantage	Main limitation / Reporting need
Gravimetric / titrimetric	Water and dissolved extracts	Low to moderate	No	Low	Simple infrastructure; useful for high concentrations	Low sensitivity; time-consuming; strong operator dependence
UV-Vis spectrophotometry	Water and digested extracts	Moderate	Limited	Low to moderate	Fast and practical for screening	Matrix interferences; reagent and pH dependence
AAS	Water, sediment, soil after digestion	Moderate to high	Generally single-element	Moderate	Reliable routine target-metal analysis	Limited throughput; requires digestion and QA/QC reporting
ICP-OES	Water, sediment, soil, and biota after digestion	High	Yes	High	Rapid multi-element routine analysis	Spectral/matrix interferences; high operating cost
ICP-MS	Water, sediment, soil, and biota after digestion	Very high	Yes	Very high	Trace and ultra-trace detection	Expensive; requires expertise, contamination control, and validation
XRF / pXRF	Soil and sediment	Moderate	Yes	Moderate to high	Rapid, non-destructive, field-applicable screening	Weaker at low concentrations; requires laboratory confirmation for risk decisions

Machine Learning and Artificial Intelligence

Applications

Machine learning and artificial intelligence-based approaches have become increasingly used as analytical tools in recent years for monitoring heavy metal pollution and assessing its ecological risk. This trend is based on the fact that heavy metal behavior in environmental systems has a multidimensional and complex structure. Metal accumulation in sediment is shaped by the combined effect of numerous variables such as lithological properties, particle size distribution, organic matter content, pH, redox conditions, hydrodynamic processes, land use, and pollutant inputs. Therefore, data-driven models capable of revealing nonlinear relationships, variable interactions, and complex patterns are needed to explain heavy metal distribution and risk patterns. Indeed, current studies show that machine learning algorithms offer a more powerful analytical framework than traditional statistical approaches in areas such as resource allocation, concentration estimation, spatial pattern analysis, and ecological risk assessment (Haque et al., 2025).

The most commonly used machine learning algorithms in heavy metal research include Random Forest, artificial neural networks, support vector machines, XGBoost, and other boosting-based ensemble models. These algorithms stand out for their ability to work with high-dimensional datasets, model multivariate interactions, and adapt to both regression- and classification-based problems. Particularly in sediment pollution studies, these models are effectively used not only in estimating metal concentrations but also in determining risk categories, separating pollutant sources, and identifying sensitive areas. In this respect, machine learning moves heavy metal research from a purely descriptive level to a more predictive and explanatory analytical level (Haque et al., 2025).

For machine learning results to be comparable across studies, performance should be reported according to the modeling task. In regression-based concentration prediction, commonly reported metrics include the coefficient of determination (R^2), root mean square error (RMSE), mean absolute error (MAE), and residual bias. In classification-based ecological risk prediction, accuracy alone is insufficient; precision, recall, F1-score, specificity, receiver operating characteristic area under the curve (ROC-AUC), and confusion matrices are needed, particularly when risk classes are imbalanced. For hotspot mapping and spatial prediction, performance should also be evaluated with spatially independent validation or station-based cross-validation rather than only random train-test splitting.

One of the significant advantages of machine learning-based models is that they do not limit input data to only metal concentrations. On the contrary, these approaches allow for the evaluation of variables that represent the environmental system in a multifaceted way within the same model. In sediment studies, variables such as pH, temperature, dissolved oxygen, electrical conductivity, salinity, organic matter, particle size, cation exchange capacity, precipitation, runoff characteristics, land use, population pressure, and geographical location are often included in the model. This approach not only reveals the current level of pollution but also identifies the key environmental drivers that drive metal accumulation. Such an approach not only describes the current state of heavy metal pollution but also explains under what conditions pollution intensifies and in which areas the risk tends to increase (Wang et al., 2024).

Applications developed specifically for sediments demonstrate that machine learning has strong potential, particularly in coastal, lacustrine, and fluvial systems. Studies on coastal sediments have shown that hybrid neural networks and boosting models can exhibit high performance in predicting metals such as arsenic and zinc. Similarly, models developed for fluvial sediments have yielded effective results in terms of metal (loid) source separation, pollution pattern classification, and probabilistic ecological risk assessment. These findings demonstrate that machine learning is not only a tool for concentration estimation but also an important decision support mechanism for determining risk priorities and shaping environmental management strategies (Yaseen et al., 2024; Li et al., 2025).

Another significant contribution of machine learning approaches is their ability to more effectively evaluate the spatial and temporal dimensions of heavy metal data. While traditional statistical methods are often limited to calculating specific indices and making comparisons between stations, machine learning models can perform pattern recognition, hotspot identification, risk classification, and future scenario prediction on larger datasets. This is especially important in matrices representing long-term environmental memory, such as sediment. The distribution of metals accumulated in sediment reflects not only current pollutant inputs but also past impacts. Therefore, machine learning offers the possibility of evaluating sediment data not only as an indicator of accumulation but also as a source of information that helps predict future environmental risk trends. In this context, machine learning has become one of the fundamental methodological tools accelerating the transition from descriptive to predictive analysis in heavy metal studies (Izah & Ogwu, 2026).

The application value of this approach is not limited to academic analysis. Machine learning-based models also provide significant advantages in terms of early warning systems, risk mapping, resource prioritization, and environmental management planning. These models are particularly functional in coastal areas, lake basins, and river networks with numerous sampling stations, helping to identify regions requiring priority intervention. Furthermore, systems integrated with real-time or semi-real-time monitoring data can contribute to earlier detection of pollution trends and more targeted planning of monitoring programs. This transforms machine learning from merely a statistical tool into a direct component of environmental decision-making processes (Izah & Ogwu, 2026; Haque et al., 2025).

However, the reliability of machine learning applications largely depends on the quality of the data used and the robustness of the modeling process. Insufficient sample size, incomplete or unbalanced data structures, inconsistencies in measurement protocols, and weak quality control practices can significantly limit model performance and generalizability. Similarly, the black box nature of some algorithms can make it difficult to correlate model results with environmental processes. Therefore, machine learning should not be considered a standalone solution replacing classical environmental analyses, but rather an integrated approach that requires consideration along with robust sampling design, reliable analytical measurement, appropriate variable selection, and careful validation processes. The literature also highlights the lack of high-quality training data, the risk of overfitting, and the limited transferability of models to different fields of study as fundamental problems in this area (Haque et al., 2025).

Furthermore, the recent rise of interpretable machine learning and explainable artificial intelligence approaches has made it necessary to evaluate not only prediction performance but also model transparency in heavy metal risk studies. Tools such as SHAP, feature significance analysis, and partial dependence curves reveal which environmental variables the model relies on for its decisions, enhancing its environmental interpretive power. However, high-performance values can be misleading if issues such as station- or time-based data leakage, spatial autocorrelation, and lack of independent validation are not controlled for. Therefore, in environmental applications, model success should be evaluated not only by accuracy measures but also by generalizability, interpretability, and external validation capacity. Table 3 presents a comparative summary of machine learning applications in heavy metal risk assessment across different ecosystems, matrices, target variables, input features, commonly used algorithms, and principal objectives.

A critical limitation in the current literature is that some studies report high model performance without sufficiently explaining data splitting, hyperparameter tuning, or external validation. This is problematic in aquatic sediment datasets because nearby stations and repeated seasonal observations may be spatially or temporally autocorrelated. If observations from the same station or campaign are distributed across both training and test sets, model performance can be artificially inflated. Therefore, transparent validation design, uncertainty reporting, and interpretable outputs should be considered minimum reporting requirements for machine-learning-supported heavy metal risk assessment.

Prediction Process: From Data Flow to Model Evaluation

The machine learning-based risk prediction process begins with the organization of data obtained from reliable sampling and analytical measurements. In this stage, metal concentrations determined from sediment and water samples, physicochemical variables, spatial coordinates, seasonal observations, and, if applicable, land use or hydrodynamic indicators are combined into a common data structure. However, the true foundation of model success is laid in the data preprocessing stage before the algorithm (Haimerl & Reich, 2025). Managing missing observations, outlier control, variable scaling requirements, class imbalance, transformation needs, and target variable definition should be clearly stated in this stage (Lin et al., 2025).

In the second stage, the dataset is divided into training, validation, and test subsets, and the selected algorithm is trained on this structure. For a robust study design, a single training-test separation should not be considered sufficient; cross-validation, external validation, or testing with independent datasets should also be used whenever possible. Since the risk of overfitting is particularly high in environmental datasets, it is essential to clearly report which hyperparameter optimization method was used, which performance metrics were preferred, and how the model's reproducibility was ensured (Öztekin & Özyılmaz, 2025).

The third stage is model evaluation and interpretation. The selected metrics should match the prediction objective. For regression models, R^2, RMSE, MAE, mean bias error, and residual plots are appropriate for evaluating concentration or risk-score prediction. For classification models, accuracy should be accompanied by precision, recall, specificity, F1-score, ROC-AUC, and a confusion matrix, particularly when high-risk observations are rare. However, reporting high-performance values alone is insufficient. Authors should explain

which variables drive the model, whether errors are concentrated in particular stations or seasons, and how the predictions relate to ecological risk processes. Therefore, feature ranking, partial dependence curves, SHAP values, and other explainable artificial intelligence tools are particularly important in studies intended to support environmental decision-making (Mallick et al., 2025).

This workflow can be adapted to different applications, from short-term monitoring studies to long-term risk analyses. However, since station-based dependence, temporal autocorrelation, and unbalanced sample distribution are common in environmental datasets, it is critical to clearly state the validation strategy used when reporting model performance (Ma et al., 2025). In particular, the uncontrolled distribution of observations from the same station or the same period to training and test sets can artificially produce high success rates. Therefore, a good predictive model only becomes meaningful with highly representative sampling, standardized analytical measurement, careful data splitting strategies, and independent validation. The machine learning process should therefore be considered as a holistic methodological chain, starting with data collection and extending to the production of interpretable and validated decision support (Taloba & Matoog, 2025). As shown in Table 4, each stage of the machine learning workflow involves specific methodological risks and requires transparent reporting of key analytical elements.

Table 3. Comparative summary of machine learning applications in heavy metal risk assessment

Ecosystem	Matrix	Target variable / output	Common input variables	Common algorithms and metrics	Main purpose and validation focus
Coastal systems	Sediment	Pb, Cd, As, Zn, Hg concentrations; hotspot classes	Metal concentrations, grain size, organic matter, salinity, pH, coordinates	Random Forest (RF), artificial neural networks (ANNs), XGBoost, hybrid models; R^2/RMSE/MAE or F1/ROC-AUC	Pollution-pattern recognition and risk hotspot identification; spatially independent validation is recommended
Lakes and reservoirs	Sediment	Total heavy metal load; ecological risk index	Precipitation, temperature, cation exchange capacity, land use, organic matter, pH	RF, support vector machines (SVMs), boosting models; R^2/RMSE/MAE for risk-score prediction	Source analysis and seasonal risk prediction: validation should control temporal autocorrelation
River systems	Sediment and water	Metal(loid) profile; ecological risk categories	Flow velocity, suspended solids, dissolved oxygen, population, and industrial pressure	RF, SVMs, ANNs; accuracy, precision, recall, F1-score, confusion matrix	Source apportionment and probabilistic risk assessment: upstream-downstream split testing is preferable
Basin-scale studies	Multiple matrices	Risk score; spatial classification	GIS layers, remote sensing indicators, climate variables, land use	XGBoost, RF, deep learning; ROC-AUC, F1-score, spatial prediction error	Early warning and decision-support systems: external validation across sub-basins is required

Table 4. Machine learning workflow and model reporting checklist

Stage	Main task	Critical risk	Elements to be reported
Data collection	Sampling and laboratory measurement	Low representativeness and contamination	Number of stations, time, depth, analytical method
Preprocessing	Missing data, outliers, scaling	Incorrect data structure	Cleaning approach and transformations
Feature selection	Preparing variables for the model	Irrelevant or redundant variables	Input variables used and selection rationale
Model training	Algorithm setup and learning	Overfitting	Algorithm type, hyperparameters, training-validation scheme
Validation	Cross-validation, independent testing, and spatial/temporal splitting	Overoptimistic performance due to leakage or autocorrelation	Split strategy, CV type, independent test data, and uncertainty
Interpretation	Explaining important variables and model behavior	Black-box outcomes and weak process interpretation	Feature importance, SHAP values, partial dependence, and ecological explanation
Reporting	Presentation of results	Lack of methodological transparency	Data source, code, uncertainty, and limitations
Performance evaluation	Selecting metrics according to task type	Incomplete or misleading performance reporting	Regression: R^2, RMSE, MAE; classification: accuracy, precision, recall, F1-score, ROC-AUC, confusion matrix

Figure 2 presents a conceptual workflow for sediment heavy metal risk prediction, demonstrating the progression from analytical measurement to interpretable decision support through preprocessing, model training, validation, and interpretation stages.

Advantages, Limitations, and Critical Evaluation

The most significant advantage of machine learning applications in heavy metal pollution studies is their ability to process large and multidimensional datasets and reveal complex relationships in environmental systems more effectively than classical methods. Heavy metal accumulation and transport often cannot be explained by a single pollutant input alone. These processes are shaped by the combined influence of geological structure, grain size, organic matter, pH, redox conditions, hydrological regime, land use, meteorological variables, and anthropogenic pressures. Therefore, models that can capture nonlinear relationships and interactions between variables offer a significant analytical advantage, especially in sediment and aquatic ecosystem studies. Indeed, current reviews show that machine learning has become a powerful tool in metal pollution research in areas such as source differentiation, concentration estimation, risk classification, and spatial pattern identification (Haque et al., 2025; Izah & Ogwu, 2026).

Another important advantage of these approaches is their ability to integrate seasonal and geographical differences into the analysis. While traditional assessments often rely on comparing concentrations measured at specific stations, machine learning models can work with multivariate environmental data to explain the spatial and temporal variation of risk in more detail. This is particularly important in dynamic systems such as coastal areas, river basins, and lake sediments (Binetti et al., 2025). This is because pollutant behavior in these ecosystems depends not only on current discharges but also on seasonal flow variations, sediment transport, erosion processes, and hydrological conditions. A recent study on lake sediments shows that evaluating multifactorial environmental variables together with machine learning-based predictive models provides more explanatory results about the sources and distribution of heavy metal pollution (Wang et al., 2024).

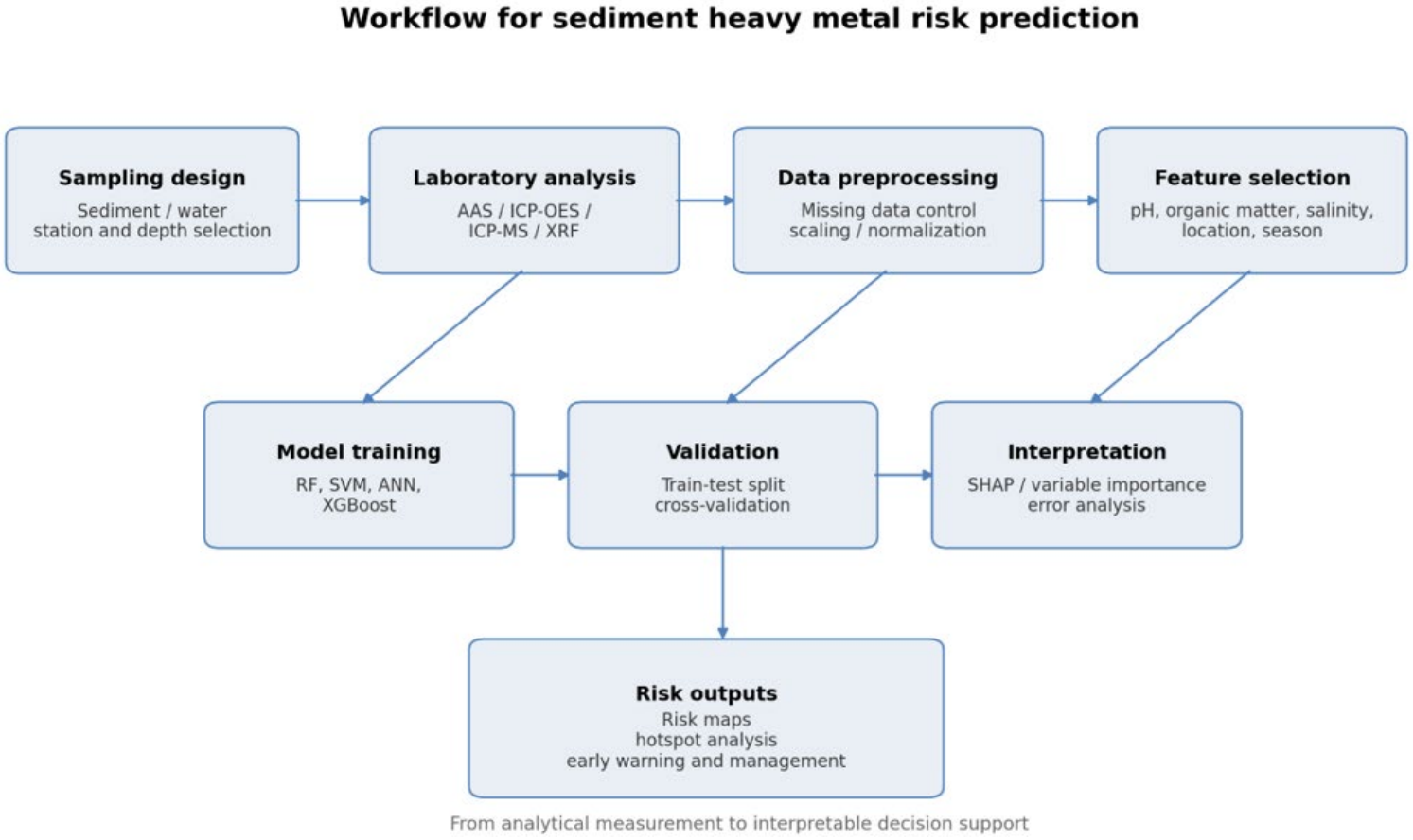

Figure 2. Workflow for sediment heavy metal risk prediction from sampling to decision support (created by the authors based on Hossain et al., 2024, and Haque et al., 2025)

One of the most notable contributions of machine learning to environmental management is that it provides a suitable foundation for early warning systems, risk mapping, and scenario-based assessments. Especially in monitoring networks with numerous stations, these models offer significant advantages in identifying areas requiring priority intervention and predicting future pollution trends (Pang et al., 2025). Instead of merely describing the current state of heavy metal pollution, predicting where it may concentrate in the future makes environmental decision-making processes more targeted and preventative. In this respect, machine learning is considered not only a tool for academic analysis but also a functional tool for determining conservation priorities and allocating resources more effectively (Izah & Ogwu, 2026).

However, the success of these models directly depends on data quality. Insufficient sample size, incomplete or unbalanced data structure, erroneous measurements, inconsistent data from different field protocols, and weak quality control processes can seriously weaken model performance (Zhao et al., 2025). Particularly in sediment and water studies, differences in elements such as sampling time, depth, grain size fraction, sample preparation method, and analytical measurement technique make it difficult for the same algorithm to achieve similar success in different studies. This clearly demonstrates that the results of machine learning models depend not only on the power of the algorithm but also on the representational power of the training data and the production of standardized data. Current literature also points to the lack of high-quality training data and data heterogeneity as the main limitations of this field (Haque et al., 2025).

Another significant limitation is the issue of generalizability across different ecosystems and study areas. A model developed in a particular lake basin, coastal system, or river sediment may not perform equally well in another region (Gohari et al., 2025). This is primarily because the environmental variables controlling heavy metal accumulation differ from ecosystem to ecosystem. As the geological background, hydrodynamic structure, land use, anthropogenic pressures, and climatic characteristics change, the patterns learned by the model also change. Therefore, a model that performs strongly at the local scale cannot be assumed to have universal validity. This point is one of the fundamental methodological problems that machine learning applications in environmental sciences must address carefully and necessitates testing models with independent datasets (Izah & Ogwu, 2026).

Furthermore, algorithm selection, hyperparameter optimization, feature selection, and interpretation of outputs require specific technical expertise. The choice between Random Forest, support vector machines, artificial neural networks, or boosting algorithms should be determined not only by accuracy criteria but also by data structure, sample size, interpretability requirements, and research objective (Wang et al., 2025). However, many studies in the literature do not report the model-building process in detail, nor do they adequately explain the hyperparameter settings, cross-validation strategies, or error measures used. This reduces the reproducibility and comparability of the studies. Current methodological discussions emphasize that the focus should be not only on higher prediction performance but also on explainability and interpretability (Haque et al., 2025; Izah & Ogwu, 2026).

From a critical perspective, the limited open data sharing, insufficient methodological standardization, and lack of long-term monitoring data in the literature are noteworthy. Heavy metal pollution studies often rely on short-term sampling campaigns. However, understanding the true dynamics of pollution in sediment and aquatic systems requires datasets that encompass multi-year and seasonal variations (Parwate, 2025). The lack of open data makes it difficult for models to be tested by independent research groups and transferred to different fields. Similarly, differences in sampling density, station selection, laboratory protocols, and risk index calculation methods also hinder direct comparison of studies. Consequently, the inability to establish a common data architecture and a common risk assessment framework in the literature limits the full integration of machine learning-based results into institutional decision-making mechanisms (Haque et al., 2025; Izah & Ogwu, 2026).

Therefore, while machine learning applications offer a powerful opportunity in heavy metal research, it is not accurate to consider them a sufficient solution on their own. For reliable results, a highly representative sampling design, standardized analytical measurement, an explainable modeling approach, independent validation, and as much open data sharing as possible should be considered together (Das, 2025). The future development of this field seems to depend not only on the use of more complex algorithms but also on the widespread adoption of explainable artificial intelligence, multi-center data sharing, long-term monitoring networks, and standardized reporting frameworks. In this context, machine learning offers a promising methodological breakthrough in environmental heavy metal risk assessment, but its true potential can only be realized with a strong database and methodological transparency (Haque et al., 2025; Izah & Ogwu, 2026).

Knowledge Gaps and Research Priorities

The reviewed literature indicates several persistent knowledge gaps. First, many studies remain based on short-term or single-season sampling, which limits the ability to

distinguish temporary hydrological effects from long-term accumulation trends. Second, differences in sampling depth, sediment grain-size fraction, digestion procedures, and analytical quality-control reporting reduce comparability among studies. Third, sediment quality indices are frequently applied without sufficient consideration of local geochemical background, mineralogy, organic matter, or sediment-water remobilization processes. Fourth, machine learning models are often developed on small or spatially clustered datasets, and their reported performance may be weakened by random validation schemes, data leakage, limited uncertainty analysis, and poor transferability to other aquatic systems.

Future research should therefore prioritize standardized sampling and reporting protocols, paired water-sediment-biota monitoring, long-term open datasets, and benchmark model comparisons across different ecosystems. Machine-learning-supported risk assessment should move toward spatially and temporally independent validation, explicit reporting of performance metrics, open code and data when possible, and stronger integration of explainability tools with environmental process interpretation. These priorities would make heavy metal risk assessment more reproducible, comparable, and useful for management decisions.

Conclusion and Future Perspectives

Overall, heavy metal analysis has undergone a significant transformation over the last half-century, moving from classical chemical methods to advanced atomic and plasma-based spectrometric techniques, and then to data-intensive and predictive analytical approaches. This transformation has not only increased measurement accuracy but has also changed the way environmental data is interpreted. Today, sediment quality assessment no longer relies solely on the quantitative determination of metal concentrations; it also includes a holistic interpretation of this data in the context of resource allocation, bioavailability, spatial patterns, temporal trends, and ecological risk. In particular, the combined use of machine learning, geostatistics, and contemporary risk assessment frameworks has paved the way for a new analytical approach that can not only describe the current state of heavy metal pollution but also predict its future trends (Haque et al., 2025; Izah & Ogwu, 2026).

Within this new approach, sediment retains its importance as a fundamental matrix representing environmental memory. This is because metals accumulating in sediment reflect not only instantaneous pollutant inputs but also long-term transport and accumulation processes. Therefore, the current trend is towards multi-layered monitoring systems that evaluate sediment data together with water column, basin characteristics, and biological responses. In recent years, the increase in studies that address water and sediment interaction together has made the need for ecosystem-scale assessment of heavy metal risk more visible. This suggests that in the future, heavy metal studies will move away from single-matrix-based approaches and towards more integrated sampling and modeling designs (Izah & Ogwu, 2026).

One of the most notable developments from a future perspective is the integration of big data infrastructures with geographic information systems, remote sensing, and machine learning models within the same analytical framework. Open-access satellite data and GIS-based spatial analyses enable the monitoring of pollutants not only through point measurements but also over wider areas and a temporal continuum. In particular, the combination of open data sources such as Sentinel and Landsat with machine learning in remote sensing water quality monitoring studies is considered a significant development that increases monitoring accuracy and area coverage. Similarly, explainable machine learning approaches not only offer high predictive performance but also enhance environmental interpretive power by making visible the variables on which the model bases its decisions. In this respect, model transparency and interpretability are expected to become one of the key quality criteria, as well as predictive accuracy, in future heavy metal research (Zhao et al., 2025).

However, certain structural requirements must be met for these developments to produce reliable and comparable results. Without open data sharing, standardized sampling protocols, consistent analytical quality control processes, and long-term monitoring networks, the generalizability of the results produced by advanced modeling approaches will remain limited. Current reviews reveal that data heterogeneity, short-term sampling designs, and reporting discrepancies create significant methodological problems in environmental metal pollution studies. Therefore, in the future, a priority should be not only developing more complex algorithms but also establishing more transparent, reproducible, and shareable data ecosystems (Haque et al., 2025; Izah & Ogwu, 2026).

In conclusion, integrating traditional environmental analysis infrastructure with machine learning and AI-supported models stands out as a powerful, feasible, and future-proof approach for monitoring and managing heavy metal risk in coastal and inland water sediments. However, for this approach to generate real scientific and managerial value, it depends on the simultaneous provision of robust analytical measurement, highly representative sampling design, interpretable modeling, independent validation, and standardized data sharing. Therefore, the future of this field lies not only

in developing more advanced devices and more complex algorithms, but also in structuring environmental data in a more holistic, transparent way that provides more direct input to decision-makers. As presented in Table 5, modern machine learning-supported approaches offer clear advantages over classical methods in terms of sensitivity, analytical scope, automation, and predictive capacity, although they also introduce challenges related to data quality and generalizability.

Table 5. A brief comparison of classical approaches and modern, machine-learning-supported approaches

Dimension / Aspect	Classical approaches	Modern / Machine-learning-supported approaches
Sensitivity	Low to moderate; limited for trace and ultra-trace levels	High to very high when supported by AAS, ICP-OES, ICP-MS, or validated XRF datasets
Scope of analysis	Limited and mostly single element	Multi-element, multivariate, and spatially explicit analysis
Data processing	Manual, slower, and operator-dependent	Automation-supported, high-throughput, and suitable for large datasets
Risk prediction	Limited; mainly descriptive or threshold-based	Strong potential for prediction, hotspot mapping, early warning, and decision support
Validation requirement	Mainly analytical calibration and recovery checks	Analytical QA/QC plus train-test design, cross-validation, external validation, and uncertainty analysis
Interpretability	Mechanistically transparent but narrow in scope	Potentially powerful but requires SHAP, feature importance, and ecological process interpretation
Main limitations	Low sensitivity, slow processing, and limited element coverage	Dependence on data quality, representativeness, transferability, and transparent reporting

Compliance with Ethical Standards

Conflict of interest: The author(s) declare no actual, potential, or perceived conflict of interest for this article.

Ethics committee approval: This study did not involve human participants or animals. The research adhered to the principles of scientific research and publication ethics.

Data availability: No datasets were generated or analyzed outside the submitted manuscript because this study is a review article.

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