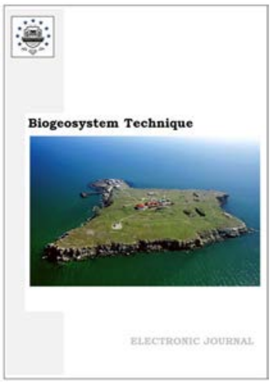
Published in the USA
Biogeosystem Technique
Issued since 2014.
E-ISSN: 2413-7316
2025. 12(2): 98-103

DOI: 10.13187/bgt.2025.2.98
https://bgt.cherkasgu.press



Short-Term Forecasting of Heavy Metal Concentrations in Soil: A Case Study of Some Regions of Armenia

Patrik Yesayan [a, *]

[a] National Polytechnic University of Armenia, Yerevan, Armenia

Paper Review Summary:
Received: 2025, November 12
Received in revised form: 2025, November 27
Acceptance: 2025, November 29

Abstract

The article examines the potential of forecasting methods to evaluate changes in the concentration of lithophilic chemical elements in soil samples, with a focus on scenarios in which limited monitoring data are available. The analysis is based on averaged chemical element concentrations, which enables assessment of the overall direction of change without reference to individual sampling points. This approach facilitates comparisons among elements, thereby allowing the identification of discrepancies in their temporal dynamics. The forecasts indicate that the concentrations of certain elements (Rb, Zr) remain unchanged, whereas those of others (Ba, Sr) show directional change or increased variability. It is imperative to account for this when interpreting pollution dynamics in the absence of detailed spatial data.

Keywords: heavy metals, artificial intelligence, machine learning, linear regression, exponential smoothing.

1. Introduction

The existing geochemical classification of chemical elements is based on their physicochemical properties, which are crucial to the formation of various geochemical systems (Perelman, 1989). However, the modern cycle of substances, exacerbated by anthropogenic environmental interventions, has become an irreversible geochemical factor in chemical migration. It is primarily due to the geochemical composition of the earth's surface. Actually, heavy metals are significant soil pollutants because they tend to accumulate and migrate through the soil over long periods (Gantulga et al., 2023; Sukiasyan et al., 2022). However, analyzing certain elements is difficult because they occur at trace and ultra-trace concentrations on the soil surface. Nonetheless, they form the foundation for the life and functioning of all biogeocenosis, from soils to living organisms. Lithophile elements stand out among these, mainly found in poorly soluble forms with low mobility and minimal participation in quick geochemical reactions (Isaev et al., 2025). Their behavior in soils mainly depends on the mineral makeup of parent rocks and overall geochemical conditions, rather than on local pollution sources. (Du Laing et al., 2009; Chougong et al., 2021).

* Corresponding author
E-mail addresses: patyesayan@gmail.com (P. Yesayan)

Consequently, it is essential to develop practical methods for controlling and monitoring environmental pollution, since data gaps often result from technical challenges in selecting and implementing geochemical techniques for these investigations (Sokolov et al., 2016).

In this context, employing artificial intelligence (AI) and machine learning (ML) models is crucial for real-time spatiotemporal environmental monitoring. This method addresses environmental challenges by handling diverse and often incomplete ecological data and integrating information on air, water, and soil quality assessments (Jordan et al., 2015; Xu et al., 2025). ML provides a more versatile and insightful analytical platform than traditional statistical methods, particularly for analyzing complex nonlinear relationships in geochemical systems (Shamsoddini, Esmaeil, 2023). ML also enables correction of anomalous values, identification of spatial trends, extraction of informative features, and improvement in the reliability of models for predicting the concentrations of chemical elements in natural environments (Ma et al., 2024; Alotaibi, Nassif, 2024).

One significant benefit of ML is its ability to automatically identify subtle data patterns and make predictions without requiring predefined functional dependencies, thereby enhancing the robustness of environmental modelling amid high uncertainty (Hao et al., 2023). Integrating ML methods into environmental research is especially crucial for evaluating soil pollution, as these datasets exhibit complex spatiotemporal patterns and are influenced by various natural and human-made factors (Gunal et al., 2023).

The article aims to address the practical challenge of enhancing environmental monitoring through AI and ML forecasting, particularly for assessing changes in soil chemical element concentrations when monitoring data are scarce.

2. Materials and methods

Soil samples were collected to a depth of 20 cm using the “envelope” method and non-metallic tools under dry-weather conditions. Target lithophile elements, including Zr, Sr, Rb, and Ba, were selected for analysis of soil from various regions in Armenia. Element concentrations were measured in the laboratory following standardized procedures (Sukiasyan, Kirakosyan, 2024). The sampling coordinates are listed in Table 1.

Table 1. Geographic coordinates of generalized sampling sites

Sampling sites		North	West
Hrazdan region	H1	40°33'04.9"	44°44'42.1"
	H2	40°33'10.4"	44°44'46.5"
	H3	40°33'29.2"	44°44'43.2"
Gavar region	G1	40°20'29.0"	45°12'22.6"
	G2	40°20'23.2"	45°12'16.8"
Martuni region	M1	40°13'49.8"	45°12'17.1"
	M2	40°13'48.5"	45°12'06.0"

The forecast model was built using data collected during a three-year monitoring period (2021–2023). These empirical data provided the foundation for modelling temporary fluctuations in concentrations. To ensure that forecasts of metal concentrations were physically realistic, a logarithmic transformation was applied before modelling. Specifically, the natural logarithm of the concentration values was computed as:

$$z_t = \log(y_t) \tag{1}$$

where y_t is the observed concentration at year t; z_t is the transformed value.

Two methods were used to model the temporal dynamics of Zr, Sr, Rb, and Ba concentrations: linear regression (LR) and exponential smoothing with a decaying trend (ETS) (Hyndman, Koehler, 2002; Koyande, 2024). LR was used to assess the trend direction (e.t, model the metal concentration as a linear function of time), and ETS was used to determine whether the trend was downward or stabilizing, extended to 2026:

$$\hat{z}_{t+k} = \beta_0 + \beta_1 x_{t+k} \tag{2}$$

where: $\hat{z}_{t+k}$ is the future values of concentration in log-space at year x_{t+k}; β_0 is the intercept; β_1 is the slope (rate of change over time).

The final predicted concentration can be calculated by:

$$\hat{y}_{t+k} = \exp(\hat{z}_{t+k}) \quad (3)$$

ETS is a state-space model. An additive error with an additive damped trend configuration is commonly applied for non-seasonal, short-term environmental data.

$$\hat{z}_{t+k} = l_{t-1} + \Phi b_{t-1} + \varepsilon_t \quad (4)$$

$$l_t = l_{t-1} + \Phi b_{t-1} + \alpha\varepsilon_t \quad (5)$$

$$b_t = \Phi b_{t-1} + \beta\varepsilon_t \quad (6)$$

where $\hat{z}_{t+k}$ is the future values of concentration in log-space at year x_{t+k}; ℓ_t is the level; b_t is the damped trend; ϕ is the damping parameter ($0 < \phi < 1$); α, β are smoothing parameters; ε_t is the forecast error.

The final predicted concentration can be calculated by:

$$\hat{y}_{t+k} = \exp(\hat{z}_{t+k}) \quad (7)$$

3. Results and discussion

Lithophile elements are the main sources of rock-forming minerals in Earth's crust (Lozovik et al., 2020). They exist as stable ions that form compounds with silicon and oxygen, such as silicates and oxides. These ions influence hydrolysis, oxidation-reduction, complexation, and precipitation in water, aiding the transfer of ions from water to soil (Alekin, Lyakhin, 1984). Soil samples collected annually from 2021 to 2023 were analyzed for Zr, Sr, Rb, and Ba. Table 2 shows the concentrations of these chemical elements in the grouped soil samples by year of collection.

Table 2. Concentration of the study lithophile element in soil sample

Sampling sites	Zr			Sr			Rb			Ba		
	2021	2022	2023	2021	2022	2023	2021	2022	2023	2021	2022	2023
H1	192.1	211.3	141.5	400.1	485.2	383.7	70.6	73.1	51.4	395.2	549.1	436.3
H2	335.3	228.2	211.0	468.2	396.5	359.8	77.7	63.9	53.6	477.4	447.2	570.7
H3	212.9	286.5	212.0	498.1	472.8	347.0	71.2	71.2	48.2	476.1	465.8	495.1
G1	186.7	184.3	147.0	527.4	565.0	515.3	60.8	57.7	41.6	436.3	537.8	578.9
G2	177.9	179.5	148.5	540.0	604.3	557.3	56.9	53.8	38.2	438.0	471.7	581.7
M1	173.3	179.4	132.1	381.1	408.5	341.7	73.4	68.8	50.2	284.3	393.4	382.3
M2	191.4	175.1	120.7	386.1	381.1	377.8	72.4	66.4	52.3	408.9	404.9	367.1

Then, to ensure reproducibility of the forecasting process, the numerical parameters of both predictive models (LR and ETS) are presented in Table 3.

Table 3. Comparison of parameters of both models: linear regression (LR) and exponential smoothing with a decaying trend (ETS)

Chemical element	LR model		ETS model				
	Intercept, β_0	Slope, β_1	Level	Trend	Damping	Initial Level	Initial Trend
Zr	286.41	-0.14	5.39	-0.14	0.995	209.94	-2.99
Sr	112.04	-0.05	6.16	-0.05	0.995	457.29	17.53
Rb	434.65	-0.21	4.29	-0.21	0.995	69.00	-3.00
Ba	-152.64	0.08	6.05	0.11	0.800	416.60	60.78

Figure 1 shows projected changes in soil concentrations of Zr, Sr, Rb, and Ba through 2026. Specifically, it presents a 95 % confidence interval for LR and a ±10 % uncertainty range for ETS.

Regarding Zr, the data up to 2023 show slight year-to-year variation, as seen in the simulation results. Subsequently, the LR model suggests a nearly flat trend through 2026, whereas the ETS model offers a smooth continuation of observed patterns with minor fluctuations. Throughout the forecast, the confidence intervals for both models remain narrow and only slightly widen over time. Finally, the comparable widths of these intervals indicate low uncertainty and strong agreement between the models for Zr, consistent with its chemical inertia and incorporation into soil silicate phases.

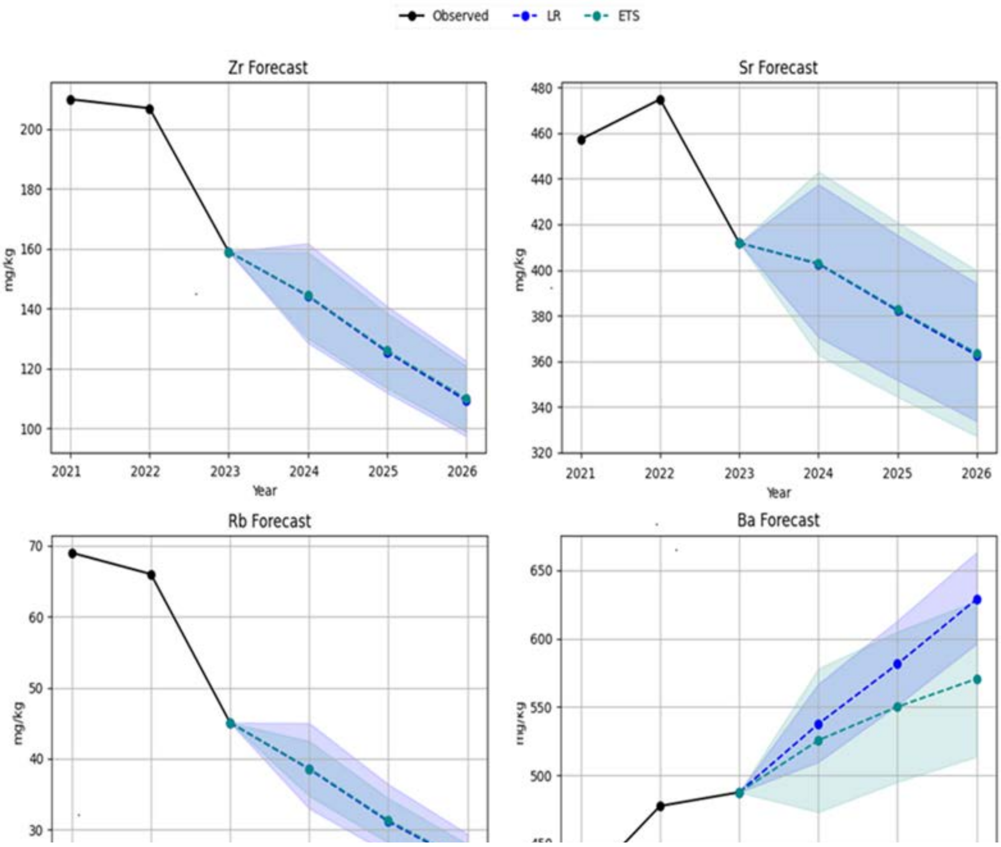


Fig. 1. Forecast of Zr, Sr, Rb, and Ba concentrations in soils through 2026 using linear regression (LR) and exponential smoothing with a decaying trend (ETS)

For Sr, LR suggests a weak directional trend that is consistently projected through 2026, indicating a modest expected change if current drivers persist. In contrast, ETS provides a smoother trajectory, signaling stability by actively preserving the present concentration level. The confidence intervals for both models gradually widen over the forecast period, a typical result of extrapolation, though they stay within observed value ranges. LR's slightly wider intervals compared to ETS's suggest this method is more responsive to year-to-year concentration variability, making it suitable for identifying shifts tied to short-term changes. This pattern reflects Sr's chemical behavior, such as its susceptibility to isomorphic calcium substitution and involvement in slow ion-exchange processes, meaning model outputs track the potential influence of these known mechanisms.

For Rb, the LR trend is very weak, with forecast values staying near the series' mean, suggesting no notable directional change under current conditions. The ETS model further flattens these dynamics, reinforcing an interpretation of long-term stability. Consistently narrow confidence intervals for both LR and ETS indicate little forecast uncertainty or expected change, which aligns with Rb's well-established fixation in potassium-rich soil minerals and amplifies confidence in status quo predictions.

For Ba, the predicted results also show high stability. LR produces a smooth, steady forecast. ETS smooths the dynamics, avoiding extremes. The confidence intervals for Ba widen only slightly and are similar across models. This shows moderate forecast uncertainty. The pattern reflects Ba's stable geochemical behavior, linked to carbonate and exchange forms. These results support using these predictions without accounting for regional differences. Building on this consistency, it is useful to examine how model behavior compares for short-term soil sample changes.

Short-term changes in soil sample concentrations were estimated using aggregated, non-spatial data. For Ba, both the LR and ETS models showed similar forecast directions and consistent trends. However, LR responded more to small, interannual fluctuations and produced more variable forecasts. ETS projections were more conservative, showing lower uncertainty over longer horizons. For lithophile elements, smoothing models like ETS are best, while LR supplements by gauging the overall trend.

4. Conclusion

Harnessing AI- and ML-based forecasting has unlocked new insights into spatiotemporal changes in lithophile element concentrations. When time-series data are limited, rely on ETS for a comprehensive assessment. For elements tightly bound to soil minerals and exhibiting low mobility, aggregated forecasting sharpens interpretation by highlighting stable background trends. Crucially, increasing model complexity or spatial detail yields only a slight improvement in forecast quality here. Ultimately, as our study affirms, align your model choice with both the data's statistical properties and the chemical characteristics of the elements.

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