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Empirical Distribution-Based Kriging Calibration for Mapping Threshold Concentration Exceedance Zones

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SUMMARY

Spatial modeling of surface water contamination is an important component of environmental monitoring and enables the identification of areas where pollutant concentrations exceed established threshold values. Kriging is one of the most widely used geostatistical methods for constructing continuous spatial models from discrete observations. However, its results are highly dependent on model and spatial search parameters, and inappropriate parameter selection may lead to overestimation or underestimation of the areas where threshold concentrations are exceeded. The study proposes an approach to calibrating Ordinary Kriging parameters based on the empirical distribution of the input data. Statistical analysis is used to determine the empirical proportion of observations exceeding the established threshold value, which serves as an independent reference indicator. Calibration is performed by comparing this indicator with the proportion of the exceedance area derived from spatial interpolation using different model parameters and by minimizing the deviation between them. Application of the proposed approach to hydrochemical datasets with different spatial sampling densities demonstrated a significant dependence of the estimated exceedance areas on spatial search parameters. It was shown that parameters can be identified for which the spatial modeling results are most consistent with the empirical characteristics of the input dataset. The proposed approach provides a formalized procedure for Kriging calibration, reduces subjectivity in parameter selection, and improves the reliability of mapping threshold concentration exceedance zones in surface water environmental monitoring.

Keywords: Kriging; Spatial interpolation; Parameter calibration; Empirical data distribution; Threshold concentrations; Surface waters; Environmental monitoring.

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Introduction

Geoinformation technologies and spatial interpolation methods are widely used in environmental monitoring systems to assess the spatial distribution of pollutants in natural environments. These methods are particularly important for surface water studies, where source data are typically represented by discrete sampling locations, whereas environmental assessment requires the construction of continuous spatial models. Geostatistical methods account for the spatial structure of observations and are widely applied to model the distribution of heavy metals and trace elements in surface water and groundwater (Rafiee et al., 2019; Wen et al., 2022; Zaresefat et al., 2024).

Ordinary Kriging is one of the most widely used geostatistical methods of spatial interpolation. It accounts for spatial autocorrelation in the input data and enables the construction of continuous surfaces from discrete measurements. However, the accuracy and spatial structure of the resulting model strongly depend on the characteristics of the input dataset and interpolation parameters. Important factors include sampling density, variogram parameters, spatial search radius, and the number of points used to estimate values at unsampled locations. Previous studies have shown that variations in sampling density and spatial search parameters can substantially affect prediction accuracy and the configuration of the interpolated surface (Dash et al., 2024; Wen et al., 2022).

This issue is particularly important when mapping threshold concentration exceedance zones. Changes in Kriging parameters may result in excessive surface smoothing or fragmentation of local anomalies and, consequently, in overestimation or underestimation of the areas where established threshold values are exceeded. Traditional statistical criteria for evaluating interpolation accuracy, including RMSE and MAE, characterize prediction errors for individual values but do not always directly reflect the reliability of delineating exceedance areas (Hodson, 2022).

Therefore, a task-oriented criterion directly related to the objective of spatial analysis is required. The aim of this study is to develop and test an approach to Kriging parameter calibration based on the empirical statistical distribution of the input data to improve the reliability of spatial assessment of threshold concentration exceedance zones in surface waters.

Method

To test the proposed approach, data from two hydrochemical surveys of surface waters were used. The datasets differ in survey scale, number of sampling locations, and sampling density (Table 1). The characteristics of the source data and the general principles of their geoinformation modeling have been described in detail in previous studies (Klypa & Karpinskyi, 2025; Klypa et al., 2025). The use of two datasets with different spatial sampling densities allows the robustness of the proposed approach to be assessed under different levels of spatial data availability.

Table 1. *Main characteristics of the hydrochemical datasets*

No.	Years	Number of samples	Survey scale	Sampling density, km	Chemical components	Units
1	1985–1988	264	1:1000000	100±20	Ba, Co, Cr, Cu, Mn, Mo, Ni, Pb, Sr, Ti, V, Zn	mg/L
2	1991–1993	560	1:500000	41±5		mg/L

Manganese (Mn) was selected as the target trace element, as both datasets contain a representative set of analytical data for this element.

At the first stage, the statistical distribution of Mn concentrations was analyzed for each dataset. Histogram analysis was used to determine the proportion of samples in which the Mn concentration exceeded the established threshold value of 15 mg/L. This indicator was denoted as P_{hist} and used as an independent empirical characteristic of the input dataset that does not depend on the spatial interpolation method or its parameters.

Ordinary Kriging was used to construct continuous spatial models. The method accounts for spatial autocorrelation between observations, while its results depend, among other factors, on the spatial density of the input data and model parameters (Dash et al., 2024; Zhang et al., 2015). Interpolation was performed using SAGA GIS tools integrated into the QGIS environment. To ensure comparability of the results, all modeling parameters, except for the tested Maximum Search Distance, were kept constant throughout the experiments: pixel size — 200 m, influence radius — 7,000 m, minimum number of points — 6–7, maximum number of points — 20–25, and number of lags — 12. A local spatial search mode and a linear variogram model with a limited correlation range were used. The Maximum Search Distance was the primary variable parameter, and its effect on the spatial modeling results was evaluated through a series of computational experiments.

For each parameter configuration, the resulting raster model was binarized according to the threshold concentration. Cells exceeding the threshold were assigned a value of 1, while all other cells were assigned a value of 0. The binarized raster was then used to calculate the total exceedance area and its proportion of the study area, denoted as $P_{kriging}$.

Model calibration was performed by comparing $P_{kriging}$ with the empirical exceedance proportion P_{hist}. To quantitatively assess the agreement between these indicators, the relative deviation function was used:

$$\boldsymbol{E} = \frac{\left|\boldsymbol{P}_{\mathbf{kriging}} - \boldsymbol{P}_{\mathbf{hist}}\right|}{\boldsymbol{P}_{\mathbf{hist}}}$$

where E is the relative deviation between the empirical and modeled exceedance proportions.

The optimal Kriging parameter configuration was defined as the one that minimized E. Thus, the calibration procedure focuses not only on the accuracy of concentration predictions at individual locations but directly on the target objective of the study — reliable delineation of threshold concentration exceedance zones.

Results

The results of a series of computational experiments confirmed a significant dependence of the estimated threshold concentration exceedance areas on the spatial search parameters. The $P_{kriging}$ values for both datasets varied substantially depending on the Maximum Search Distance (Table 2).

Table 2. *Results of Kriging parameter calibration and values of the relative deviation function E*

No.	***Search Distance (m)***	***$P_{kriging}$ 1985-1988***	***P_{hist} 1985-1988***	***E 1985-1988***	***$P_{kriging}$ 1991-1993***	***P_{hist} 1991-1993***	***E 1991-1993***
1	10 000	1.16	24.28	0.952	15.55	34.65	0.551
2	15 000	12.68	24.28	0.478	33.35	34.65	0.038
3	17 000	20.91	24.28	**0.139**	35.35	34.65	**0.020**
4	20 000	31.69	24.28	0.305	36.75	34.65	0.061

Analysis of the results showed that, for both datasets, the minimum value of the relative deviation function E was achieved at a Maximum Search Distance of 17,000 m. For the 1985–1988 dataset, the minimum value was E=0.139, whereas for the denser 1991–1993 dataset it was E=0.020. Thus, despite differences in survey scale and sampling density, the best agreement between the spatial interpolation results and the empirical distribution was obtained at the same spatial search parameter value (Figure 1).

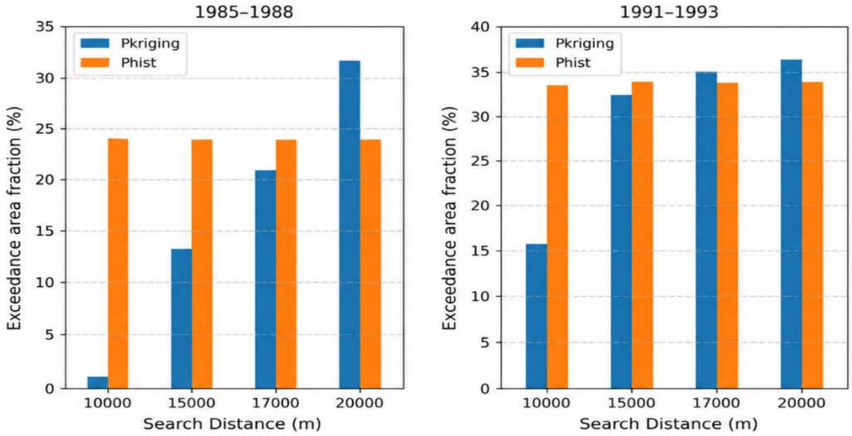

Figure 1. *Comparison of the proportion of the Mn threshold concentration exceedance area obtained by Kriging ($P_{kriging}$) with the empirical value determined by histogram analysis (P_{hist}) at different Maximum Search Distance values*

Analysis of the spatial configuration of the resulting zones confirmed the quantitative calibration results. For the 1991–1993 dataset, at a Maximum Search Distance of 10,000 m, the interpolated surface was characterized by considerable fragmentation and high local variability. Increasing the search distance to 15,000 m resulted in a more spatially connected structure of the exceedance zones. At 17,000 m, a spatial configuration of the exceedance zones was obtained for which the deviation between the modeled area proportion and the empirical indicator was also minimal. A further increase in the search distance to 20,000 m resulted in excessive smoothing and enlargement of the exceedance zones (Figure 2).

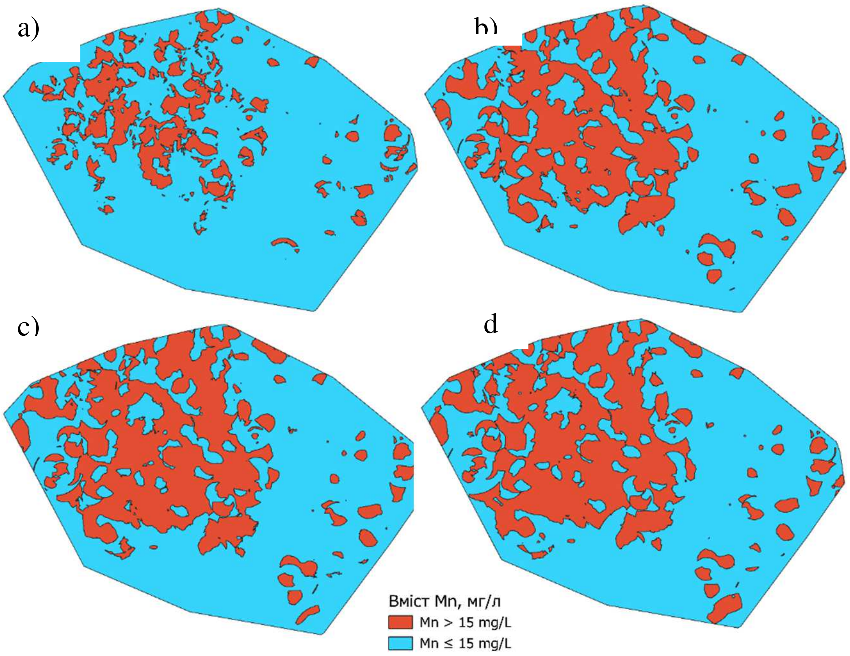

Figure 2. *Spatial configuration of Mn threshold concentration exceedance zones for the 1991–1993 dataset at different Maximum Search Distance values: a — 10,000 m; b — 15,000 m; c — 17,000 m; d — 20,000 m*

The results demonstrate that the proposed criterion enables quantitative identification of the spatial search parameter at which the interpolation results are most consistent with the empirical characteristics of the input data. The lower E value obtained for the denser dataset also indicates greater stability of geostatistical modeling under conditions of higher spatial sampling density, which is consistent with previous findings on the effect of sampling density on the accuracy of Ordinary Kriging (Dash et al., 2024).

Conclusions

The study confirmed the significant influence of spatial search parameters on Ordinary Kriging interpolation results and the estimation of threshold concentration exceedance areas. Changes in the Maximum Search Distance were shown to result in either fragmentation of the spatial structure and underestimation of exceedance areas or excessive surface smoothing and their overestimation.

The proposed calibration approach, based on comparing the proportion of the exceedance area obtained by Kriging with the empirical proportion of exceedances in the input dataset, provides a formalized procedure for model parameter selection. For two datasets with different spatial sampling densities, the minimum value of the deviation function was obtained at the same Maximum Search Distance, while the denser dataset demonstrated greater stability of the modeling results.

Using the empirical distribution as a task-oriented criterion complements traditional accuracy metrics and enables the geostatistical model to be evaluated directly in terms of the reliability of delineating threshold concentration exceedance zones. The proposed approach can be applied in GIS-based environmental monitoring of surface waters and further tested for other hydrochemical components and datasets with different spatial structures.

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