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Spatial Interpolation of the Probability of Mercury Threshold Exceedance using Indicator Kriging

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Abstract

icator Kriging (IK) is a spatial interpolation method used to estimate the probability that a variable exceeds a specified threshold. This study applies IK to assess the probability of mercury (Hg) concentrations exceeding environmental thresholds in river systems across DKI Jakarta. Given the skewed and non-normally distributed nature of mercury data, IK was selected due to its robustness in handling non-parametric data and its sensitivity to extreme values. Mercury concentration measurements were first transformed into binary indicator data based on a predefined threshold. An experimental semivariogram was then computed to analyze the spatial dependence of the indicator values, followed by the fitting of theoretical semivariogram models (Gaussian, Spherical, and Exponential). The best-fitting model was selected using the Leave-One-Out Cross-Validation (LOOCV) approach, with the Spherical model yielding the lowest root mean square error (RMSE). The final probability map generated through IK reveals five unsampled locations with a probability greater than 0.5 of mercury concentration exceeding the threshold: two located along the Ciliwung River and three along the Sunter River. These findings highlight critical zones requiring monitoring and support the use of IK as an effective geostatistical tool for environmental risk assessment of heavy metal contamination in urban river systems.

Keywords: *Indicator Kriging, Mercury, Spatial Interpolation*

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1. INTRODUCTION

Geostatistics is a statistical discipline that explicitly accounts for the spatial dependence and structure inherent in georeferenced data [1]. Geostatistics encompasses several methods, one of which is spatial interpolation. Spatial interpolation is a technique used to estimate the values of unmeasured locations for a field variable within the spatial extent of the sampled area [2]. Kriging and Inverse Distance Weighted (IDW) are two of the most commonly used spatial interpolation methods [3]. Each of these methods has its own advantages. Inverse Distance Weighted (IDW) can estimate values more quickly due to its simpler conceptual framework, whereas the Kriging method provides an estimation of error variance, allowing researchers to assess the accuracy of the predicted values.

The Kriging and IDW methods are frequently compared in various studies for value estimation due to their similar underlying concepts. Several studies have compared these two methods, including research conducted by Sanusi, which demonstrated that the Kriging method produced better results than the IDW method in estimating rainfall data in South Sulawesi [4]. The Kriging method with a Gaussian semivariogram produced a lower RMSE compared to the IDW method. A similar study conducted by Luo supports this finding, showing that the Kriging method produced more accurate estimations than the IDW method [5]. This study also demonstrated that the Kriging method resulted in a lower RMSE compared to the IDW method. Based on several studies comparing Kriging and IDW, it can be concluded that the Kriging method tends to provide more accurate estimation results than the IDW method.

Kriging interpolation includes several advanced methods such as Universal Kriging, Co-Kriging, Indicator Kriging, and others. Indicator Kriging is one of the extensions of Ordinary Kriging, designed for non-stationary data and variables with binary or categorical scales. Unlike Ordinary Kriging, Indicator Kriging offers greater flexibility, as it can estimate the probability of exceeding a specified threshold for data that are non-stationary, non-normally distributed, and contain extreme values. Moreover, Indicator Kriging reduces sensitivity to outliers since it utilizes binary-transformed data [6]. The concept of Indicator Kriging is to estimate the probability of exceeding a certain threshold, rather than directly predicting exact values as in Ordinary Kriging. Therefore, the estimation results from Indicator Kriging and Ordinary Kriging cannot be directly compared. However, considering the flexibility in handling various types of data, Indicator Kriging is a suitable solution for estimating exceedance probabilities in datasets that are not appropriate for use with the Ordinary Kriging method [7].

In the Indicator Kriging method, the semivariogram is used to determine the spatial structure and to calculate the appropriate estimation weights prior to performing the analysis [8]. Based on their formation, semivariograms are classified into two types: experimental semivariograms and theoretical semivariograms [9]. The experimental semivariogram is constructed from observed data and visualized in a graph, while the theoretical semivariogram serves as a reference model to fit the experimental semivariogram. Several theoretical semivariogram models can be used, with the most commonly applied being the Gaussian, Spherical, and Exponential models [10]. These theoretical semivariogram models have distinct characteristics, making them suitable for different types of data and spatial situations. The selection of an appropriate theoretical semivariogram model is crucial, as it can significantly affect the accuracy of the spatial analysis results.

Water is one of the most essential natural resources for human life and all other living organisms [11]. Rivers are one of the surface water resources on Earth. Humans typically utilize rivers for various purposes such as water storage, transportation, irrigation, fish farming, and recreation. In some regions of Indonesia, rivers are even used for daily activities such as bathing and washing [12]. Jakarta is a city where a portion of the population still relies on rivers for daily activities such as bathing and washing. According to data from Badan Pusat Statistik DKI Jakarta in 2022, approximately 25% of residents living along riverbanks continue to use river water for their daily needs. This issue warrants serious attention, as a 2023 report by Dinas Lingkungan Hidup DKI Jakarta indicated that around 78% of rivers in Jakarta are classified as heavily polluted. One of the primary reasons river water is deemed unsuitable for bathing and washing is the high concentration of mercury (Hg) found in many of these water bodies [13]. The use of water containing high concentrations of mercury (Hg) can lead to numerous health problems in humans, including infertility, impaired motor function, reduced muscle strength, various skin disorders, and other serious conditions [14].

This spatial interpolation method was chosen because mercury (Hg) concentration data in Jakarta's rivers are spatial in nature, taking into account the geographic location of each observation point. The probability of mercury presence in Jakarta's rivers can be effectively assessed using one of the spatial interpolation techniques, namely Indicator Kriging. This method was selected because estimating the probability of mercury presence is essential for supporting the Jakarta city government's policymaking, particularly in regulating the use of river water for activities such as bathing and washing, as well as for guiding further research on mercury contamination in Jakarta's river water.

2. RESEARCH METHOD

2.1. Method

In this study, the method to be used is the Kriging spatial interpolation method. Kriging is a method developed by D.G. Krige for estimating the values of mineral deposits. It shares a similar conceptual framework with the IDW method, as both estimate values within a sample area using a linear combination of weights. The key assumption of the Kriging method is the presence of spatial correlation among the sample data [15]. Ordinary Kriging is the simplest form of Kriging in geostatistics. This method assumes stationarity in the spatial data, with an unknown but constant mean across the study area [16]. Indicator Kriging serves as a solution to the limitations of Ordinary Kriging, which assumes data normality and is not capable of providing probability estimates for the presence of a variable at a specific location [17]. In practice, Indicator Kriging transforms continuous data into discrete binary values of 0 and 1. Although it is often described as a non-linear method, Indicator Kriging is, in fact, a linear Kriging technique applied to non-linear, transformed data [17].

Before applying Indicator Kriging, the continuous variable data $z(s)$ is transformed into discrete indicator data $\omega(s)$ using following formula:

$$\omega(s) = \begin{cases} 1, & If\ z(s) \geq z_c \\ 0 & Others \end{cases} \tag{1}$$

After the data is transformed into a binary (discrete) form, the analysis using the Indicator Kriging method can begin. The transformed data can then be estimated using the following Indicator Kriging equation 2:

$$\hat{\Omega}(s_0) = \sum_{i=1}^{N} \lambda_i \omega(s_i) \tag{2}$$

with:

$\hat{\Omega}(x_0)$ = Estimated indicator value at the target location, representing the probability of exceeding the specified threshold.

$\omega(x_i)$ = Indicator value at the i-th sample location, derived from the mercury concentration data based on Equation (1).

λ_i = Kriging weight assigned to the i-th sample, obtained from the indicator semivariogram model.

s_0 = Target location to be estimated

s_i = Location of the i-th sample point

N = Number of sample points used in the estimation

Since Indicator Kriging is the simplest extension of Ordinary Kriging, the weighting process is carried out in the same manner as in Ordinary Kriging. Indicator Kriging produces an estimator that is linear, unbiased, and has minimum variance. With these three properties, Indicator Kriging is referred to as a Best Linear Unbiased Estimator (BLUE) [18].

Kriging interpolation is performed only after the experimental semivariogram has been properly fitted to a theoretical semivariogram model. The goodness of fit between the experimental and theoretical semivariograms can be assessed using cross-validation methods [19]. Cross-validation is used to evaluate the assumptions of the experimental semivariogram and assess how well it fits the chosen theoretical semivariogram model along with its parameters [20]. Rather than simply testing for error, cross-validation serves as a more comprehensive evaluation method. Although cross-validation cannot confirm the absolute correctness of the chosen theoretical semivariogram model, it can indicate which theoretical model best approximates the experimental semivariogram that has been constructed [21]. One of the cross-validation methods that can be used to assess the fit of a semivariogram model is Leave-One-Out Cross-Validation (LOOCV). In this method, out of a total of n data points, one data point is removed and used as the test data, while the remaining $n - 1$ points are used as training data. This process is repeated for each data point. The Root Mean Square Error (RMSE) is then used to compare the accuracy of different models. The RMSE is calculated using the following formula:

$$RMSE = \sqrt{\frac{1}{N}\left\{Z(s_i) - \hat{Z}_{-i}(s_i)\right\}^2} \tag{3}$$

When the RMSE score of a model is lower, the model is considered more accurate. Conversely, a higher RMSE score indicates lower accuracy of the model.

2.2. Data

The data used in this study is secondary data on river water quality in DKI Jakarta for the year 2022. The dataset includes information collected from 23 rivers, which are, Angke, Blencong, Buaran, Cakung, Cengkareng, Cideng, Ciliwung, Cipinang, Grogol, Jati Kramat, Kalibaru Barat, Kalibaru Timur, Krukut, Kamal, Kanal Timur, Mampang, Mookervart, Pesanggrahan, Petukangan, Sekertaris, Sepak, Sunter, Tarum Barat.

A study conducted by Pandiangan stated that the observation points for mercury concentration across all rivers in Jakarta need to be increased [13]. Observation points in rivers across Jakarta need to be increased because many residents rely on these rivers as a source of water for their daily needs. The addition of observation points aims to ensure that the water used by nearby communities is safe and does not pose any health risks. The spatial distribution of both sampled and unsampled locations is illustrated in the following Figure 1. The figure illustrates the spatial distribution of water-quality sampling locations across the river network, where blue points represent sampled sites and red points denote unsampled locations used for spatial evaluation. Although many sampled points are positioned along major and minor waterways, the distribution is not uniform, with several river segments lacking direct observations. This uneven spatial coverage highlights critical data gaps and reinforces the importance of applying geostatistical interpolation techniques such as Indicator Kriging to estimate mercury concentrations at unobserved sites. The underlying administrative boundaries and river system, depicted with light blue flow lines, provide geomorphological and hydrological context for interpreting spatial patterns. Overall, the visualization forms a crucial foundation for generating continuous prediction surfaces and assessing potential mercury contamination risks across the study domain. All calculations and map visualizations in this study were performed using R software.

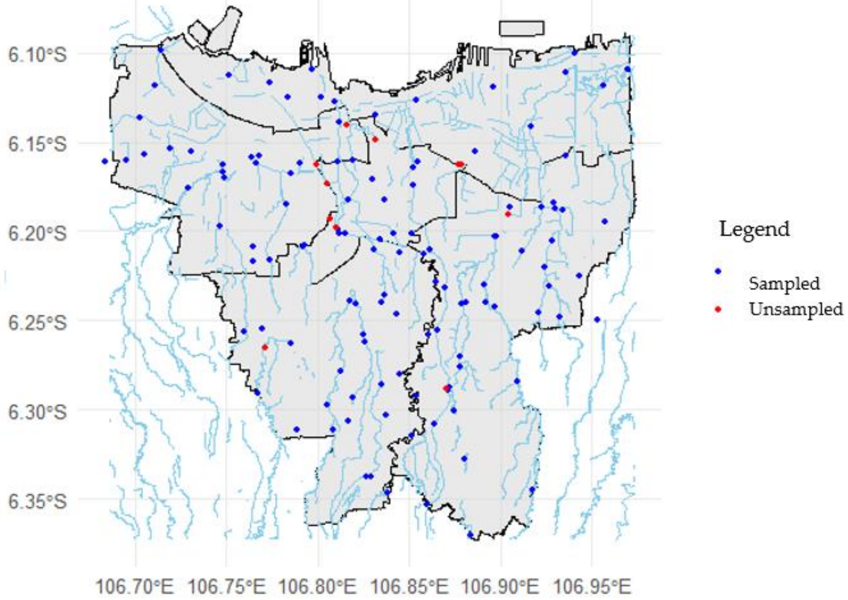


Figure 1. Spatial Visualization of Sampled and Unsampled Points

2.3. Research Procedures

The research procedures in this study are as follows:

1. Preparing mercury concentration data in river water within the Special Capital Region of Jakarta (DKI Jakarta).
2. Defining the threshold value to distinguish specific conditions.
3. Calculating descriptive statistics.
4. Transforming the original continuous data into indicator data.
5. Visualizing the spatial distribution of the indicator data on a map.

6. Constructing a semivariogram map to examine directional influence.
7. Determining the type of semivariogram based on directionality.
8. Calculating the experimental semivariogram for the indicator data.
9. Visualizing the experimental semivariogram to identify the maximum range and semivariogram shape.
10. Modeling the theoretical semivariogram based on the processed experimental semivariogram.
11. Validating the semivariogram model using the Leave-One-Out Cross-Validation (LOOCV) method.
12. Calculating the Root Mean Square Error (RMSE) to evaluate model performance.
13. Estimating indicator values at unsampled locations using the best-fitted theoretical semivariogram model.
14. Calculating the probability that the estimated values at certain locations meet specific criteria based on the indicator values.
15. Creating a spatial probability map that illustrates the likelihood of each location meeting the defined criteria.

The research flowchart is presented in **Figure 2**.

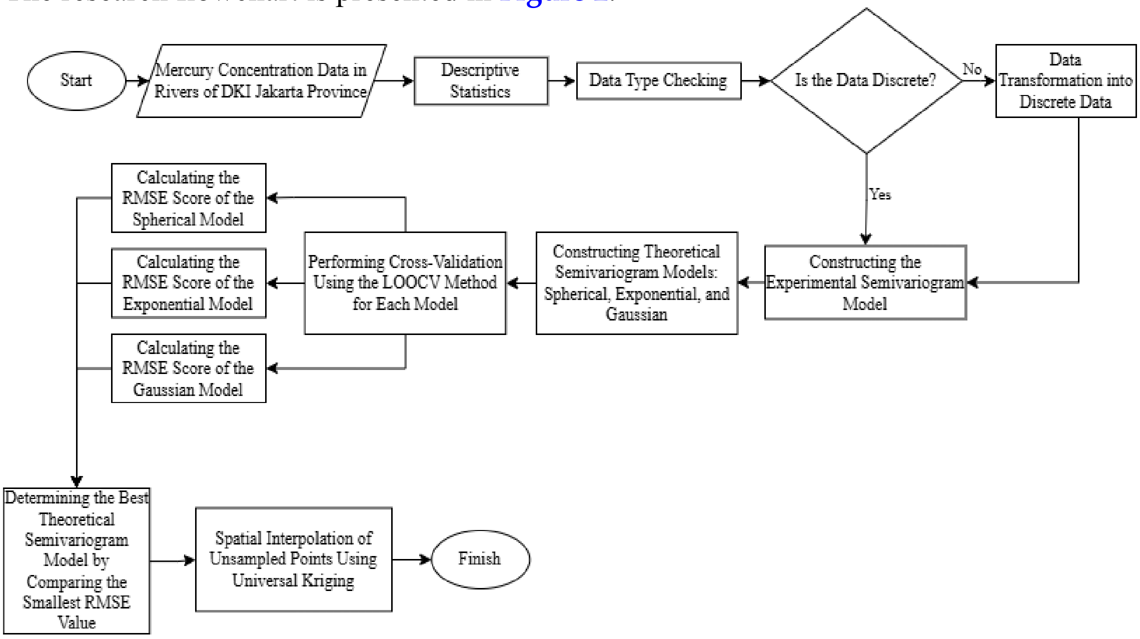


Figure 2. **Research Flowchart**

3. RESULT AND DISCUSSION

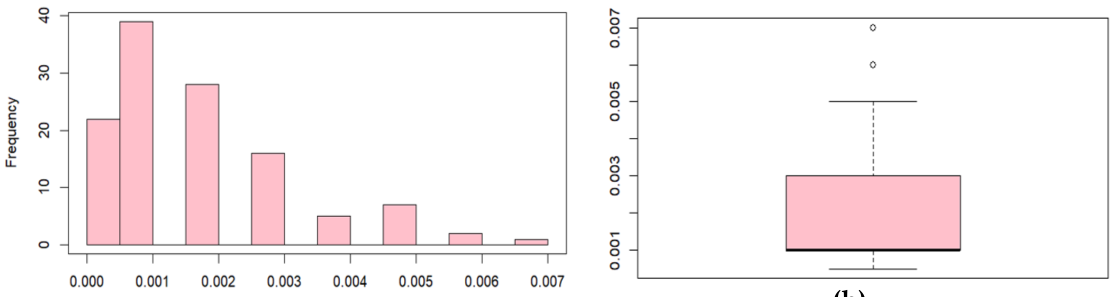
3.1. Descriptive Statistics

The descriptive statistics of mercury concentration data from 120 sampled points are presented in **Table 1** below:

Table 1. **Descriptive Statistics of Mercury Concentration at Sampled Locations**

Mean	Variance	Std. Deviation	Min	Max
0.001898	0.000002	0.001431	0.0004900	0.007000

From **Table 1**, it can be seen that the average mercury concentration at the sampled locations is 0.001898. This average indicates that the mercury concentration in Jakarta's rivers exceeds the safety threshold of 0.001. This means that, on average, the mercury content at the sampled river points in DKI Jakarta is not suitable for consumption or daily use, as it surpasses the permissible limit for mercury in water. Furthermore, the variance of the mercury concentration data is 0.000002, with a standard deviation of 0.001431. This suggests that the mercury concentration data at the sampled river points in DKI Jakarta is relatively homogeneous, as indicated by the low variance. In other words, the mercury concentrations across these locations show minimal variation and tend to be uniform. The highest recorded mercury concentration at the sampled points is 0.007 (or 0.7%), found in the Ciliwung River. This can be attributed to the high population density along the river and the lack of control over both domestic and industrial waste disposal in the surrounding area. Elevated mercury levels in the Ciliwung River can have severe health impacts on nearby communities that still rely on river water as their primary source for daily needs. On the other hand, the lowest mercury concentration, 0.00049 (or 0.049%), was found at several locations: two points in the Sekertaris River, one in the Sunter River, two in the Sepak River, two in the Krukut River, one in the Angke River, and seven points in the Mookervart River. The lower mercury levels in these rivers are likely due to the limited presence of industrial zones nearby, making it easier to control both industrial and domestic waste.



(a) **(b)**

Figure 3. Plot of Mercury Concentration (a) Histogram and (b) Boxplot

From **Figure 3(a)**, the histogram exhibits a left-skewed (negatively skewed) distribution, indicating that most observations are concentrated at lower mercury concentrations while only a small number of samples extend toward higher values. This pattern suggests the potential presence of relatively high concentration observations that may act as outliers. The boxplot in **Figure 3(b)** supports this indication, showing several upper outliers above the whiskers, which likely reflect localized contamination hotspots. The combination of skewness and the presence of outliers demonstrates that the data deviate from normality. Consequently, Indicator Kriging represents an appropriate geostatistical approach for this dataset, as it is capable of accommodating skewed distributions, mitigating bias caused by extreme values, and providing a probability-based assessment of threshold exceedance.

3.2. Experimental Semivariogram

The experimental semivariogram is constructed as an initial step in semivariogram modeling. The distance used in semivariogram calculations can be weighted by direction (anisotropy) or not (isotropy). The following is a directional semivariogram map, which is used to determine whether direction has an influence on the semivariance values.

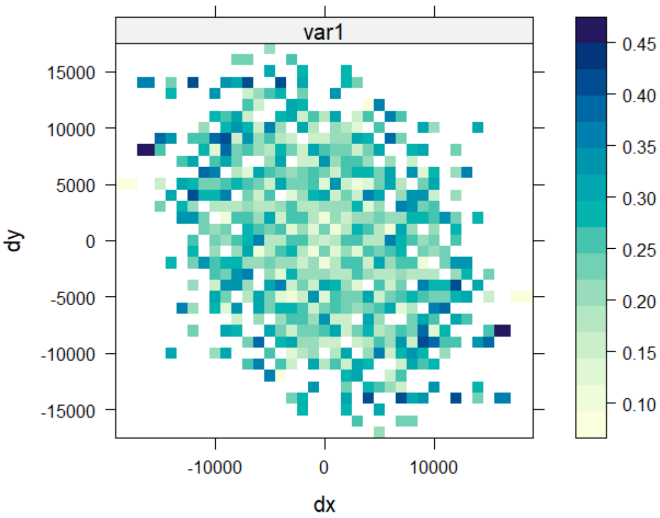


Figure 4. **Semivariogram Map**

Based on the directional semivariogram plots in **Figure 4**, there is no evidence of directional dependence in the spatial continuity of the data. The semivariance values across the examined directions exhibit similar patterns, with no direction consistently showing higher or lower semivariance than the others. This uniformity indicates the absence of spatial anisotropy. Given that the spatial dependence appears consistent in all directions, an isotropic semivariogram model is appropriate for this study. Employing an isotropic model ensures that spatial continuity is represented uniformly across the study area and aligns with the observed characteristics of the mercury concentration data. The results of the semivariogram calculation using the binning process, assisted by R-Studio software, are presented in **Figure 5**.

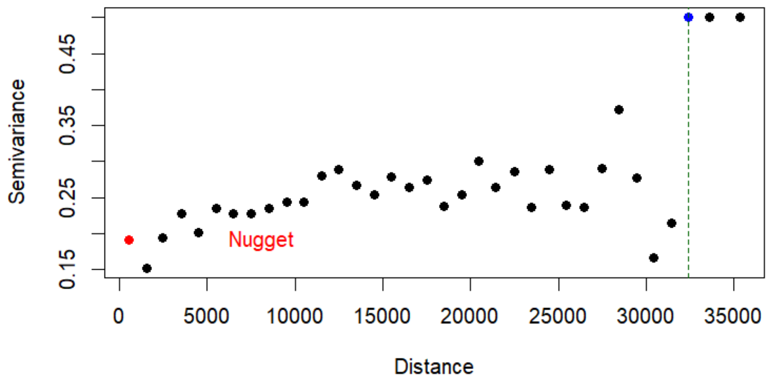


Figure 5. **Experimental Semivariogram Plot Results**

From the experimental semivariogram plot above, it can be observed that the sill is around 0.5, as there is no further increase in the semivariance values beyond this point. The range of the experimental semivariogram is approximately 30,000, as this is the distance at which the sill is reached. Additionally, the nugget effect begins at around 0.15.

3.3. Theoretical Semivariogram

Theoretical semivariograms are fitted to the experimental semivariogram to determine which model best represents the observed spatial structure. The models considered in this study are the Spherical, Exponential, and Gaussian models. The following presents the fitting of the theoretical semivariogram models to the experimental semivariogram.

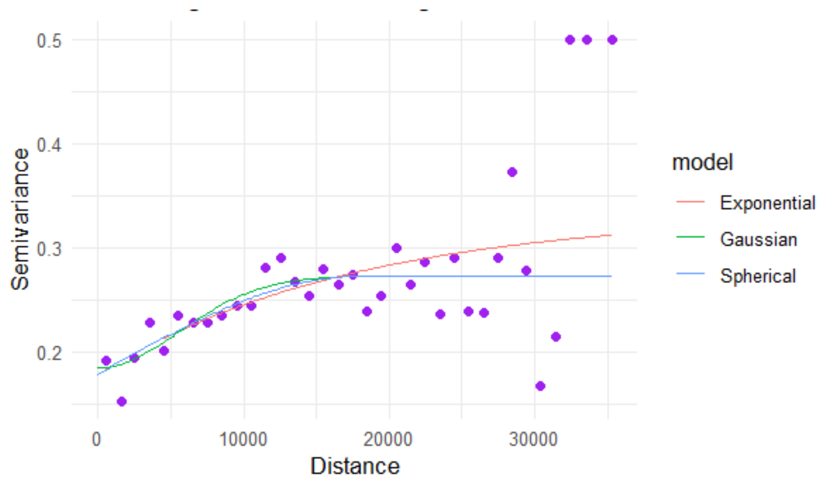


Figure 6. **Fitting of Spherical. Exponential. and Gaussian Theoretical Semivariogram Models**

From **Figure 6** above, the nugget effect, sill, and range values for each model can be obtained as follows.

Table 2. **Theoretical Semivariogram Results**

Models	Nugget Effect (C_0)	Sill($C_0 + C$)	Range (A)
Spherical	0.1	0.28	15000
Exponential	0.1	0.31	35000
Gaussian	0.18	0.28	16000

Thus, the resulting models are as follows.

- Spherical theoretical semivariogram model

$$\gamma(h) = \begin{cases} 0.28\left[\dfrac{3h}{15000} - \dfrac{h^3}{2 \times 15000^3}\right]. & if\ h \leq 15000 \\ 0.28 \quad . & if\ h > 15000 \end{cases}$$

- Exponential theoritical semivariogram model

$$\gamma(h) = 0.31\left[1 - exp\left(-\frac{h}{35000}\right)\right]$$

- Gaussian theoritical semivariogram model

$$\gamma(h) = 0.28\left[1 - exp\left(-\frac{h^2}{16000^2}\right)\right]$$

Next, to select the best theoretical semivariogram model for estimating the probability of mercury concentration exceeding the threshold, cross-validation testing is conducted using the Leave-One-Out Cross-Validation (LOOCV) method.

3.4. Cross Validation

Cross validation using the Leave-One-Out Cross-Validation (LOOCV) method is conducted to select the best theoretical semivariogram model. The evaluation metric used is the Root Mean Square Error (RMSE). Each model yields its own RMSE value represent the difference between the experimental semivariogram and the modeled semivariogram, and the best model is determined by comparing these values—specifically, the model with the lowest RMSE is selected because a lower RMSE means that the chosen model more accurately captures the spatial continuity and variability structure of the mercury indicator data. The **Table 3** below presents the RMSE values obtained from each model.

Table 3. RMSE Calculation Results for Each Model

Model	*RMSE*
Spherical	**0.4363955**
Eksponensial	0.4377296
Gaussian	0.440193

Based on **Table 3**, the RMSE calculation results for each theoretical semivariogram model can be observed. The lowest RMSE value is found in the Spherical model, which is 0.4363955. Therefore, the Spherical theoretical semivariogram model is selected for estimating the probability of mercury concentrations exceeding the threshold in rivers across DKI Jakarta.

3.5. Interpolation of Unsampled Points

After the best-fitting theoretical semivariogram model is determined, the estimation of the probability that mercury concentrations exceed the threshold at unsampled locations is carried out using the Indicator Kriging method with the Spherical semivariogram model. From the estimated probabilities, we can further analyze which locations are likely to have mercury concentrations above the threshold. A location is considered potentially exceeding the threshold if the probability is greater than or equal to 0.5. The results of the probability estimation for unsampled locations, based on the original dataset and computed using R-Studio software, are presented in **Table 4** below.

Table 4. Estimated Probability of Mercury Exceeding the Threshold at Unsampled Locations

River	Latitude	Longitude	Probability	Assumption
Ciliwung	-6.1982	106.81	0.340001	Not exceeding
Ciliwung	-6.1977	106.81	0.341632	Not exceeding
Ciliwung	-6.1927	106.8069	0.335245	Not exceeding
Ciliwung	-6.1735	106.8049	0.384503	Not exceeding
Ciliwung	-6.1407	106.8161	0.690999	Exceeding
Ciliwung	-6.1489	106.8318	0.648132	Exceeding
Angke	-6.2654	106.7712	0.265441	Not exceeding
Sunter	-6.2881	106.8706	0.936789	Exceeding
Sunter	-6.1909	106.9043	0.425379	Not exceeding
Sunter	-6.1631	106.8771	0.537241	Exceeding
Sunter	-6.1629	106.8787	0.539342	Exceeding
Cakung	-6.1629	106.7989	0.383186	Not exceeding

The following is a spatial distribution map of the estimated probability of mercury exceeding the threshold at unsampled locations.

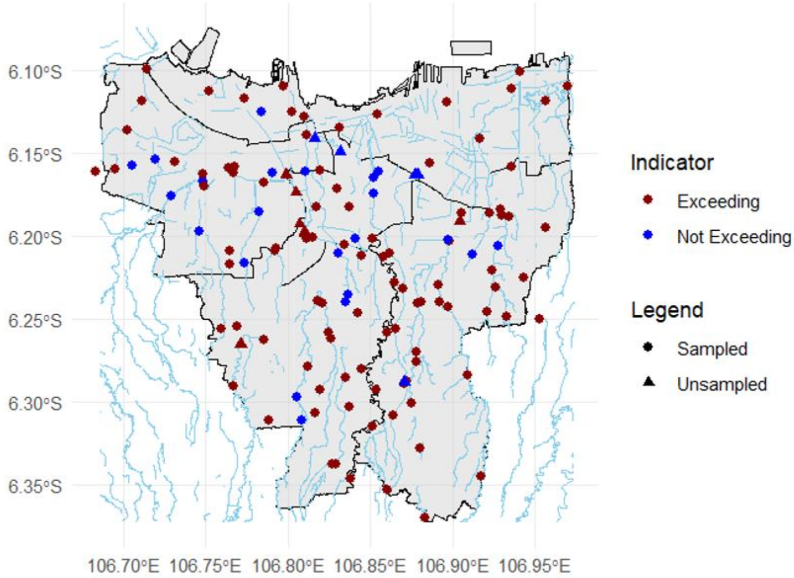


Figure 7. Estimated Probability of Mercury Exceeding the Threshold at Unsampled Locations

The estimation results at unsampled points using the Indicator Kriging method show that there are five unsampled locations with a high probability of having mercury concentrations exceeding the threshold—two points along the Ciliwung River and three along the Sunter River. This finding should be of particular concern to relevant authorities to minimize the negative impacts of river water containing mercury above safe levels. In **Figure 7**, sampled data points are represented by circles while interpolated points are represented by triangles. The spatial distribution of unsampled points visualized in **Figure 7** also shows that the estimation aligns with the conditions of nearby sampled points. This indicates that the selected theoretical semivariogram model accurately represents the spatial trend of the data. making the estimations at unsampled locations considered reliable. Furthermore, **Figure 7** reveals spatial continuity in the mercury indicator along the river flow. This suggests that the spread of mercury may be influenced by the flow of the river. Therefore, relevant institutions are encouraged to consider further analysis on the dynamics and sources of mercury pollution to develop more effective mitigation strategies.

4. CONCLUSION

The analysis concludes that the Spherical semivariogram model provides the best fit for estimating the probability of mercury concentrations exceeding the environmental threshold in DKI Jakarta rivers, yielding the lowest RMSE value (0.4364) among the models tested. Indicator Kriging successfully identified five unsampled locations, two along the Ciliwung River and three along the Sunter River, indicating areas of potential environmental concern. Statistically, the findings underscore the importance of selecting an appropriate semivariogram model and increasing the density of sampling points to reduce interpolation uncertainty. It is recommended that future studies explore a wider range of semivariogram models, including more flexible structures, to enhance model robustness. Moreover, increasing the number and spatial coverage of observation points, particularly in under-sampled areas, is essential for improving estimation accuracy. Environmental authorities are also encouraged to conduct regular monitoring and implement early warning systems in high-risk areas. Lastly, incorporating temporal analysis in future research could provide valuable insights into seasonal patterns and long-term trends of mercury pollution.

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Author Contributions Statement

Mufdhil Afta Zhahirulhaq: Conceptualization, Software Implementation, Formal Analysis, Investigation, Data Curation, Original Draft Preparation, And Visualization. Dwi Agustin Nuriani Sirodj: Conceptualization, Methodology Design, Validation, Supervision, Review and Editing of The Manuscript, and Funding Acquisition.

Conflict of Interest Statement

The authors declare no conflict of interest.

Informed Consent

None

Ethical Approval

None

Data Availability

The data that support the findings of this study are secondary data on river water quality in the Special Capital Region of Jakarta (DKI Jakarta), obtained from the Satu Data Jakarta portal for the year 2022. The dataset is openly available at the following link: https://satudata.jakarta.go.id/open-data/detail?kategori=dataset&page_url=data-kualitas-air-sungai&data_no=1.

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