Dynamical spatial model of heavy metals in Kendari bay using Bayesian geographical weighted regression

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Abstract. Kendari Bay has been designated as an ecotourism area and as the main route for local trading in Kendari City, Province of Southeast Sulawesi, Indonesia. An earlier study conducted by Armid et al [2] found that water quality in Kendari Bay has been polluted by heavy metals from household and factory wastes. Such metals are spatially distributed throughout Kendari Bay area, but the main source of contributors to pollutants has not yet been identified clearly. A study on the distribution of heavy metals in the aquatic system of Kendari Bay is imperative to determine the source and status of pollution. This study aims for analyzing the main source of the largest pollutant contributors in Kendari Bay in order to maintain the water quality in this bay. The model for analyzing spatial effect is geographical weighted regression (GWR), and Bayesian Markov Chain Monte Carlo (MCMC) is used to estimate GWR parameters. The data of this study originated from 32 sampling sites spread across the Kendari Bay area, referring to a previous study by Armid et al [2]. Based on these data, numerical simulation results were obtained with prior r = 35 and δ = 10 which produced the best BGWR model with the highest $R^2$ value of 86.75% and the lowest MSE value of 0.02290; suggesting that 86.75% of the pollutants are caused by heavy metals Pb, Cd, and Cr, while 13.25% is caused by other factors. There are two sampling sites that have significant effects on the number of pollutants in Kendari Bay, both site 3 (downstream of the Wanggu River) and site 29 (Port area).
1. Background

The dynamics of pollutants, such as heavy metals in coastal areas including bays are influenced by a number of factors such as chemical, physical, and biological interactions between freshwater and saltwater [1, 3, 4, 5, 20, 21]. The presence of heavy metals is now a serious concern because it endangers the life of coastal organisms and human health. Mining practices, industrial activities, urban development, other human activities near rivers and estuaries, as well as other biological activities have an important role in contributing pollutants in coastal areas and polluting the marine environment [3, 9, 14]. The presence of heavy metals poses serious environmental problems because it damages water quality and can be bioaccumulated in marine organisms [6, 7, 8, 9]. Therefore, the coastal region is an important geochemical component for the marine environment as a data supplier for marine pollution studies [11, 15, 16, 18].

Kendari Bay is a coastal area located in Kendari City in Southeast Sulawesi Province of Indonesia. The bay has become a center for tourism, transportation, and fisheries throughout the city's coastal areas. The bay is connected to the Wanggu River in the east and there are three large ports located in the middle of the bay which may influence the chemical characteristics of metals in the water system of Kendari bay. A study on the geochemical distribution and pollution status of heavy metals in Kendari Bay is significance required to manage water quality in the bay. The previous study of the distribution of heavy metal concentrations in Kendari Bay was conducted by [2]. They used data from 32 sampling sites ranging from the downstream area of the Wanggu River to the offshore area of Kendari Bay and determined the pollution status by comparing their data to the normal levels of metals in the oceanic waters.

The present study analyzes the data patterns of such 32 samples and taking into account the spatial influence among sampling sites. Data between sampling site are influenced by geographical environmental conditions and other human activities [10, 12]. The impact of spatial influence is shown by its parameters that vary spatially, hence the global regression becomes less able to explain the real data phenomenon [13, 17]. One of the models that can be used in terms of spatial influence is the geographical weighted regression (GWR). The Bayesian Markov Chain Monte Carlo (MCMC) approach is used to estimate the model parameters that are quite complex [19].

2. Data Description

Spatial data is the geographically oriented data since it contains information concerning attributes and locations. This data has two important parts which make it different from other data, which is location information (spatial) and descriptive (attribute). Location information (spatial) relates to a geographic coordinate, including latitude and longitude, while descriptive information (attribute) or non-spatial information has some information such as density and type of metal. The condition of an observation location (sampling site) differs from other sites. Nevertheless, the condition of each site has a close relationship with other sites that are close together [12]. The linkage between sampling sites is called the spatial heterogeneity, this happens because of the differences in environmental and geographical characteristics variations between the sampling sites. Therefore, each site has its own magnitude.

The data used in this study are the heavy metals data of Pb, Cd and Cr of Kendari Bay from the previous measurement by [2]. Kendari Bay is located at $3^\circ58'S$ and $122^\circ34'E$ with an area of $10.84 \text{ km}^2$. There are three ports located in the western part of the bay, including the Ferry Port, Perikanan Samudera Port, and Nusantara Port. Ferry Port is used as a commercial port, Perikanan Samudera Port as a fishing landing harbour, and Nusantara Port is an industrial container harbour for cargo ships. Sampling (32 sites) was carried out from the upper reaches of the Wanggu River to the outer bay connected to the Banda Sea, as shown in Figure 1. These data are used since the three heavy metals being studied are distributed along the Kendari Bay [2].
Figure 1. Map of 32 sampling sites at Kendari Bay for investigation of heavy metals Pb, Cd and Cr

Percentage of pollutants symbolized by P as the response variable and predictor variables are the concentrations (µg/L) of heavy metal Pb, Cd and Cr measured in the aquatic system of Kendari Bay at 32 sampling sites. The range, minimum, maximum, average and standard deviation values of the three predictor variables are tabulated in Table 1.

Table 1. Range, minimum, maximum, average and standard deviation values of predictor variables

| Variable       | Max. | Min. | Range | Average  | Standard deviation |
|----------------|------|------|-------|----------|--------------------|
| P (response)   | 7.39 | 0.84 | 6.55  | 3.124750 | 1.862521595        |
| Pb (predictor) | 0.549| 0.009| 0.54  | 0.2096562| 0.183976087        |
| Cd (predictor) | 0.015| 0.001| 0.014 | 0.0078750| 0.003562801        |
| Cr (predictor) | 0.386| 0.085| 0.301 | 0.1489062| 0.061463527        |

Table 1 shows that the concentration of heavy metal Pb is quite large compared to both Cd and Cr, suggesting that the distribution of Pb pollutant in Kendari Bay varies spatially. Table 1 further shows that the standard deviation of heavy metal Cd is the smallest (~ 0.004), which indicates that the distribution of Cd pollutant in Kendari Bay is heterogeneous. To strengthen the alleged spatial heterogeneity, a Breusch-Pagan test was performed. The Breusch-Pagan statistical value was obtained the chi-square value, 11,133 and the p-value, 0.01103. This specifies that there is a pattern of spatial heterogeneity regarding the spread of heavy metals Pb, Cd, and Cr Kendari Bay region. Therefore, modeling of heavy metal distribution data in Kendari Bay region should accommodate the influence of location (sampling site).

Before constructing the model, it must be ascertained that the predictor variables affect the response variable. In addition, the predictor variables must also be ensured that they are independent of each other. To demonstrate this, Pearson correlation analysis is used. The results of the Pearson correlation test are presented in Table 2.
Table 2. Results of Pearson correlation test between variables

| Variable    | Pearson correlation | p-value   |
|-------------|---------------------|-----------|
| Pand Pb     | 0.9385215           | 0.0000006516 |
| P and Cd    | -0.08800328         | 0.632     |
| Pand Cr     | 0.641752            | 0.00007535 |
| P and Cd    | -0.2360962          | 0.1933    |
| P and Cr    | 0.4544613           | 0.08974   |
| Cd and Cr   | 0.1185285           | 0.5182    |

Table 2 shows that the three predictor variables affect the response variable as the p-value less than 0.05. It is also found that all the predictor variables are independent of each other, based on p-values greater than 0.05.

3. Bayesian Geographically Weighted Regression Model

The GWR model is the development of a regression model with the assumption that the observation of each location $i$ is homogeneous, $y_i = X_i \beta_i + \epsilon_i$, where $\beta_i$ is a parameter vector at location $i$ which has size $u_i \times 1$. Meanwhile, $X$ is the data matrix of heavy metals Pb, Cd, and Cr as predictor variables and $y$ is a pollutant concentration as response variable, and $W_i$ is the weighting matrix of location $i$. Since the pollutant data is spatial heterogeneity, the GWR model is modified using the Bayes approach, the so-called Bayesian GWR (BGWR) as it is able to overcome heterogeneity cases between locations.

$$\beta_i = (w_{i1} \otimes I_k \ldots w_{in} \otimes I_k) \begin{pmatrix} \beta_1 \\ \vdots \\ \beta_n \end{pmatrix} + u_i,$$

where $w_{ij}$ is the distance weighting between locations $i$ and $j$, row vector $(w_{i1}, w_{i2}, \ldots, w_{in}) = 1$ and $w_{ii}=0$. Distribution of errors at each location $\epsilon_i$ and vector $u_i$ follow a normal distribution ($\epsilon_i \sim N(0, \sigma^2 \mathbf{v}_i)$) and $u_i \sim N(0, \sigma^2 \delta^2 (X W_i^2 X)^{-1})$. $v_i = diag(v_1, v_2, \ldots, v_n)$ as a heterogeneity vector of location $i$ and $\sigma^2$ is various errors. Vector $\mathbf{v}_i$ is a prior that has a chi-square distribution or $v_i \sim \chi^2(r)$, where $r$ is a hyperparameter as a control number of prediction distribution $\mathbf{v}_i$. This prior was used by [17] for the analysis of variance problems and [12] for heteroscedasticity and outlier models. Such prior is also utilized to modify $\mathbf{v}_i$ hence $E(\mathbf{v}_i) = 1$ and $Var(\mathbf{v}_i) = 2/r$. If $r$ value is extremely large, then the BGWR error range will be $\sigma^2 I_n$ or homogeneous and if $r$ value is quite low, then the BGWR error range will be spatially heterogeneous. The stochastic parameter $\mathbf{u}_i$ spread normally with zero mean and variance based on Zellner’s g-prior $\sigma^2 (X W_i^2 X)^{-1}$ to show the diversity of smoothing relationship parameters with $\beta_i$.

The matrix $W_i$ is the spatial weighting of location $i$ where the diagonal elements value is determined by the proximity of location $i$ to location $j$ (other location). The closer the location, the greater the weighting value on the corresponding element. One of the spatial weighting functions in BGWR is adopted from the Gauss Kernel function form $w_{ij} = \exp \left[ -\frac{1}{2} \left( \frac{d_{ij}}{b} \right)^2 \right]$, where $d_{ij}$ is the distance from location $i$ to location $j$, $d_{ij} = \sqrt{(u_i - u_j)^2 + (v_i - v_j)^2}$, and $b$ is bandwidth which is a value that describes the maximum distance of a location and still affects other locations. One of the ways to get the optimum bandwidth value is to minimize the value of $CV = \sum_{i=1}^{n} |y_i -$
\[ \hat{y}_{x_i}(b) \] which is the fitting value at location \( i \) [10]. The optimum bandwidth uses the Gaussian kernel principle obtained from the iteration process to get the minimum CV.

4. Numerical Simulation

The BWGR model parameters are estimated using the Gibbs sampler Bayesian Markov Chain Monte Carlo (MCMC). Model parameters being estimated are \( \beta_i, \sigma_i, \delta, v_i \) with the conditional posterior distribution. Posterior distribution of \( \beta_i \) with condition \( \sigma_i, \delta \) and \( v_i \) are

\[ p(\beta_i|\sigma_i, \delta, v_i) = \mathcal{N}(\tilde{\beta}_i, \sigma_i^2, \delta^2) = B(\tilde{X}_i v_i^{-1} \tilde{y}_i + \tilde{X}_i \tilde{v}_i / \delta^2) \] and \( B = (\tilde{X}_i v_i^{-1} \tilde{X}_i + 1 / \delta^2)^{-1} \). The conditional posterior distribution for \( \sigma_i \) is proportional to the exponential function \( p(\sigma_i|\beta_i, \delta, v_i) \propto \sigma_i^{-(m+1)} \exp \{ -1 / 2 \sigma_i^2 (\epsilon_i^2 v_i^{-1} \epsilon_i) \} \), where \( m \) is the number of observations. The conditional posterior distribution for \( v_i \) with chi-square distribution is:

\[ p(\sigma_i|\beta_i, v_i) \propto \delta^{-n} \exp \left\{ -\sum_{i=1}^{n} \left( \frac{1}{2} (v_i - \tilde{v}_i) (\tilde{X}_i^{-1} (\tilde{X}_i v_i^{-1} \tilde{X}_i) - 1 \beta_i - \tilde{v}_i) \right) \right\} \]

The conditional posterior distribution for \( \delta \) is also proportional to the exponential function

\[ p(\delta|\sigma_i, \beta_i, v_i) \propto \beta_i^2 \exp \left\{ -\sum_{i=1}^{n} \left( \frac{1}{2} (v_i - \tilde{v}_i) (\tilde{X}_i^{-1} (\tilde{X}_i v_i^{-1} \tilde{X}_i) - 1 \beta_i - \tilde{v}_i) \right) \right\} \]

Gibbs sampling algorithm:

1. Determine the initial values of \( \beta_i^0, \sigma_i^0, \delta^0, v_i^0, i = 1, 2, \ldots, n \)

2. For each observation \( i \)
   a. Generate \( \beta_i \) from \( p(\beta_i|\sigma_i, \delta, v_i) \)
   b. Generate \( \sigma_i \) from \( p(\sigma_i|\beta_i, \delta, v_i) \)
   c. Generate \( v_i \) from \( p(v_i|\beta_i, \sigma_i, \delta) \)
   d. Generate \( \delta \) from \( p(\delta|\sigma_i, \beta_i, v_i) \)

3. Repeat step 2 for \( m \) iterations until they reach convergent value. Convergence can be monitored through:
   1) trace plot, is a picture of a plot of iteration versus the value that has been generated. A rising or falling trend in the parameter values in the trace plot indicates that the burn-in period has not been reached. If trends like these arise, it is important to eliminate the initial part of the chain or burn-in process. Convergence is achieved if the historical plot trend is already in the same zone
   2) plot autocorrelation, convergence is achieved if the chain in successive iterations is no longer a strong correlation. If a sequential iteration process is still correlated then the information provided is only marginally concerning the target distribution and not the value of a single simulation. Autocorrelation measures the correlation between \( n \) iteration and \( n+1 \) iteration simulation values
   3) Ergodic mean plot, shows the mean up to the current iteration. If after several iterations the ergodic mean is stable, then this is an indication of the achievement of convergence

The estimated parameters of the BGWR model for the concentration of heavy metals Pb, Cd, and Cr from 32 sampling sites in Kendari bay are presented in Table 3. The testing of model parameters is used to determine the heavy metal variables that affect pollutant fluctuations at 32 sampling sites. The significance level using the t-test, at \( \alpha = 0.05 \), \( t_{(PB, Cd, Cr)} = \frac{\hat{\beta}_i}{SE(\hat{\beta}_i)} \), where \( SE(\hat{\beta}_i) \) is standard error of estimated parameters. If \( |t_{(PB, Cd, Cr)}| \geq t_{(n-p-1), 0.05} \) or \( t \) table, it
is concluded that heavy metals at location have a significant effect on pollutant fluctuations. Table 3 shows that there are two main sources of pollutant contributors (P) in Kendari Bay, i.e. sampling sites 3 and 29. Sampling site 3 is located downstream of the Wanggu River,

\[
\hat{P}_{(3)} = 0.0548 + 2.5536 \, Pb_{(3)} + 20.8937 \, Cd_{(3)} + 1.618 \, Cr_{(3)},
\]

and sampling site 29 located in the Ports area,

\[
\hat{P}_{(29)} = -0.0055 + 2.6967 \, Pb_{(29)} + 24.6645 \, Cd_{(29)} + 1.4922 \, Cr_{(29)}.
\]

### Table 3. Parameter estimation of BGWR model per sampling site

| Sampling site | Interception | Pb  | Cd  | Cr  | \(t_{Pb}\) | \(t_{Cd}\) | \(t_{Cr}\) |
|---------------|--------------|-----|-----|-----|------------|------------|------------|
| 1             | 0.0656       | 2.7034 | 6.0144 | 2.7256 | 0.204252 | 0.454411 | 0.205929 |
| 2             | 0.0478       | 2.7176 | 5.8457 | 2.4213 | 0.237449 | 0.510765 | 0.21156  |
| 3             | 0.0548       | 2.5536 | 20.8937 | 1.618  | 0.325355 | 2.647185 | 0.204997 |
| 4             | 0.0479       | 2.975  | 12.613 | 1.5263 | 0.257911 | 1.093455 | 0.132319 |
| 5             | 0.0714       | 2.5026 | 3.1154 | 3.1181 | 0.265652 | 0.330701 | 0.330987 |
| 6             | 0.0513       | 2.764  | 16.5303| 1.7313 | 0.194448 | 1.16291  | 0.121797 |
| 7             | 0.0416       | 2.8975 | 15.0188| 2.0837 | 0.228045 | 1.182043 | 0.163996 |
| 8             | 0.0454       | 2.6097 | 13.9285| 1.9985 | 0.211947 | 1.131203 | 0.162308 |
| 9             | 0.0416       | 2.8757 | 16.7597| 1.7261 | 0.290727 | 1.694371 | 0.174505 |
| 10            | 0.0512       | 2.5776 | 2.387  | 2.8463 | 0.23887  | 0.022121 | 0.263771 |
| 11            | 0.0336       | 2.5793 | 6.1551 | 2.6217 | 0.301426 | 0.719306 | 0.306381 |
| 12            | 0.0228       | 2.7275 | 6.0453 | 2.4081 | 0.191154 | 0.423679 | 0.168769 |
| 13            | 0.0063       | 2.447  | 2.0292 | 2.951  | 0.268429 | 0.225982 | 0.323717 |
| 14            | 0.0079       | 2.66   | 13.1311| 3.2852 | 0.260142 | -1.28419 | 0.321285 |
| 15            | 0.0347       | 2.9572 | 17.0878| 1.7236 | 0.188558 | 1.089561 | 0.109901 |
| 16            | 0.0151       | 2.8053 | 9.6176 | 2.1648 | 0.253181 | 0.867999 | 0.195376 |
| 17            | 0.0224       | 2.9269 | 8.8698 | 1.687  | 0.347365 | 1.05267  | 0.200214 |
| 18            | 0.0262       | 2.7392 | 18.6214| 1.9339 | 0.267197 | 1.816438 | 0.188644 |
| 19            | 0.0418       | 2.7167 | 2.2779 | 2.5912 | 0.348474 | 0.292188 | 0.332376 |
| 20            | 0.0383       | 2.8163 | 9.5624 | 2.0078 | 0.19856  | 0.674187 | 0.141558 |
| 21            | 0.0056       | 2.816  | 7.0386 | 2.3049 | 0.229881 | 0.574589 | 0.188158 |
| 22            | 0.0144       | 2.8973 | 18.332 | 1.5797 | 0.194481 | 1.230534 | 0.106037 |
| 23            | 0.0188       | 2.7826 | 12.9306| 2.1963 | 0.312399 | 1.451702 | 0.246576 |
| 24            | 0.0121       | 2.7395 | 18.9485| 1.8049 | 0.214254 | 1.481949 | 0.14116  |
| 25            | 0.0204       | 2.9054 | 13.659 | 1.6372 | 0.273908 | 1.28771  | 0.154348 |
| 26            | 0.0113       | 2.8046 | 15.2824| 1.7431 | 0.290036 | 1.629462 | 0.185855 |
| 27            | 0.0101       | 2.3444 | 2.5309 | 3.0425 | 0.189759 | 0.204855 | 0.246265 |
| 28            | 0.0132       | 2.586  | 10.7161| 2.5377 | 0.307491 | 1.274209 | 0.301748 |
| 29            | -0.0055      | 2.6967 | 24.6645| 1.4922 | 0.288066 | 2.634702 | 0.159399 |
| 30            | 0.0203       | 2.3282 | 15.4852| 2.4792 | 0.179567 | 1.19433  | 0.191214 |
| 31            | 0.0307       | 2.6285 | 12.5814| 1.7319 | 0.175899 | 0.841948 | 0.115899 |
The source of heavy metals at sampling site 3 may originate from nature and the results of human activities on land. The results of field validation at this site indicate that there has been a significant increase in development and industrial activities. Anthropogenic input is strongly suspected to have originated largely from these activities. The aquatic system of Kendari Bay, including downstream of the Wanggu River, will clearly get metals input from the land through river flow, both in the form of industrial waste and other wastes from run-off. Furthermore, site 29 is closely related to activities in the port area, such as community activities around the port and the entry and exit of large ships with various types of cargo such as petroleum and commercial goods. Waste from activities at the port is strongly suspected to have contributed to pollutants at this sampling site. The location of samplingsites 3 and 29 is shown in Figure 2.

Figure 2. Location of the main source of pollutants in Kendari Bay, sampling site 3 and site 29

5. Conclusions
Based on various priors $r$ and $\delta$ used in the analysis of the BGWR method for estimating the number of pollutants in Kendari Bay, prior $r = 35$ and $\delta = 10$ are priors that produce the best BGWR model with the highest $R^2$ value, 86.75% and the MSE value, 0.02290. The $R^2$ shows that 86.75% of the number of pollutants in Kendari Bay marine environment is caused by heavy metals Pb, Cd and Cr, while the rest is caused by other factors. There are two sampling sites that have a significant effect on the number of pollutants in Kendari Bay, i.e. sampling sites 3 (downstream of the Wanggu River) and 29 (Port area). This is alleged because anthropogenic activities around these two points can increase the number of pollutants in Kendari Bay.

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