Implementation of Ordinary Co-Kriging method for prediction of coal quality variable at unobserved locations

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Abstract. A Co-Kriging method is a method that used to predict the value of the point at unobserved locations by sample points are known to be spatially interconnected by adding other variables that have a correlation with the main variable or can also be used to predict 2 or more variables simultaneously. In this research, the Lagrange Multiplier approach is used to produce the minimum variance of the Co-Kriging estimator. The case study is predicted on coal quality variable, Fixed Carbon as the main variable with Calorific Value as an additional variable. The process of prediction calculation by Co-Kriging method using package GStat on R software which produces a best theoretical model is Gaussian model as input in the prediction calculation at unobserved locations. The calculation result with Lagrange Multiplier approach using R Program is faster, precise and accurate which produces minimum prediction variance for Fixed Carbon and Calorific Value variables.

1. Introduction

Lagrange Multiplier is a method used to determine the maximum or minimum value of a function that has constraints [1]. This method is widely used in various applied problems in the real world, one of them in the field of Geostatistics. Geostatistics is a combination of mining, geology, mathematics, and statistics that was originally developed in the mineral industry to estimate mineral deposits on Earth [2]. The use of Lagrange multipliers in the field of Geostatistics is one of them is used to minimize prediction variance in prediction method at an unobserved location, ie Kriging method [3]. The Kriging method consists of several types, namely the Ordinary Point Kriging method and Ordinary Block Kriging method which assumes the average is unknown, the Simple Kriging method which assumes the average is known and constant, the Universal Kriging method which assumes the average is known and not constant, and the Co-Kriging method which is a combination of the Kriging method [4]. Application of Ordinary Point Kriging methods is used in the prediction of pollutants on the Meuse river floodplain [5], then the predicted contours are developed with projection to google map [6], the prediction of the pollutants was developed using the Universal Kriging method [7]. Along with the development of science and technology, in this study discussed the usefulness of Kriging methods in coal mines. Some researchers have used the Kriging method, one of which is used for risk management in the coal industry [8], then used for prediction of coal quality [9], also used to predict coal seam thickness [10], and is used in predicting rock shear strength at coal mine [11].
Indonesia is a country rich in natural resources, especially mining materials. Currently, Indonesia according to the United States Geological Survey (USGS) ranked 6th as a country rich in mineral resources, apart from that of its mineral potential for coal, Indonesia is ranked 3rd [11]. According to estimates, Indonesia’s coal resources reach 18-19 billion tons, while reserves are estimated at 17-18 billion tons spread across Indonesia [11]. Some factors that affect the quality of coal, include: Volatile Matter (%), Fixed Carbon (%), Ash Content (%), Calorific Value (cal / gr), and Total Sulfur (%) [12].

Based on the above description one of the things that can be done in predicting variables that affect the quality of coal is the Kriging method [9]. Because the determinant factor of coal quality consists of five variables, the Kriging method that can be used to predict the coal quality determinant variables is the Co-Kriging method, which is a Kriging technique involving other variables [13]. For the case study, in this study used data obtained from the results of research at PT Bumi Merapi Barat Lahat South Sumatra, the variables of coal quality. One of the tools that can be used in the prediction calculation process is R software which is open source software, besides R software provides a special package in the calculation of the Kriging method is GStat package [14] and for example to illustrate the Bayesian Kriging use geoR package [15].

Research on Lagrange Multiplier approach to Co-Kriging method has been done [3], besides that research on the application of Kriging method in coal mining case has been done a lot. However, there has not been much discussing the prediction of coal quality using Co-Kriging method with calculation using R software. Therefore, this study discussed Lagrange Multiplier approach on Co-Kriging method for prediction of coal quality by using R software.

2. Method
2.1. Crossvariogram
Crossvariogram is a function of distance $h$ which denotes semi covariance between the difference of the main variables by the difference of the additional variables within $h$ [2]. Crossvariogram is used to observe a spatial correlation between the most common variables in the sample data and is used in Co-Kriging method because it involves two or more variables so that the spatial relationship of those variables can be known. Here is the equation of Crossvariogram:

$$\hat{\gamma}_{1,2}(h) = \frac{1}{2N(h)} \sum_{i=1}^{N(h)} [Z_i(x_i + h) - Z_i(x_i)][Z_i(x_i + h) - Z_i(x_i)] .$$

(1)

2.2. Theoretical Model
The most commonly used theoretical model 3 is the Spherical model, Gaussian model and Exponential model [10]:

1. Exponential model

$$\gamma(h) = c \left[1 - \exp\left(-\frac{h}{a}\right)\right].$$

(2)

2. Gaussian model

$$\gamma(h) = c \left[1 - \exp\left(-\frac{h^2}{a}\right)\right].$$

(3)

3. Spherical model

$$\gamma(h) = \begin{cases} 
1,5\left(\frac{h}{a}\right) - 0,5\left(\frac{h}{a}\right)^3, & h < a \\
c, & h \geq a
\end{cases} .$$

(4)
2.3. Ordinary Co-Kriging Method

1. Linear
Based on [13] the Ordinary Co-Kriging estimator for two variables obtained from \( n \) observation data used to form a linear model, namely:

\[
Z(x) = \sum_{i=1}^{n} \lambda_i [Z_i(x_i)] + \sum_{j} \alpha_j [Z_j(x_j)].
\]  

(5)

2. Unbiased
Based on [10] the Ordinary Co-Kriging estimator is unbiased if:

\[
E[Z(x) - Z(x)] = E\left[\sum_{i=1}^{n} \lambda_i Z_i(x_i) + \sum_{j} \alpha_j Z_j(x_j) - Z(x)\right]
\]

\[
= \sum_{i=1}^{n} \lambda_i E[Z_i(x_i)] + \sum_{j} \alpha_j E[Z_j(x_j)] - E[Z(x)]
\]

\[
= \sum_{i=1}^{n} \lambda_i \alpha_i E[Z_i(x_i)] + \sum_{j} \alpha_j E[Z_j(x_j)] - E[Z(x)]
\]

\[
= 0
\]

because the mean is assumed to be unknown then \( E[Z_i(x_i)] + E[Z_j(x_j)] - E[Z(x)] = 0 \) then the nature of the estimator can not be satisfied by the Ordinary Co-Kriging method.

3. Best
The best intent here is the Ordinary Co-Kriging estimator has the minimum estimator variance, the estimation variance of the Ordinary Kriging as follows:

\[
\sigma_{CK}^2 = \text{Var}[Z(x) - Z(x)]
\]

\[
\sigma_{CK}^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} \lambda_i \alpha_i \text{Cov}[Z_i(x_i) + Z_j(x_j), Z_i(x_i) + Z_j(x_j)] + \sigma^2 - 2 \sum_{i=1}^{n} \sum_{j=1}^{n} \lambda_i \alpha_i \text{Cov}[(Z_i(x_i) + Z_j(x_j)), Z(x)].
\]  

(6)

to obtain the minimum value of the error variance using the Lagrange Multiplier method with the Lagrange Multiplier parameter, the Lagrange Multiplier equation is expressed as follows [11]:

\[
F(\lambda_i, \alpha_j, \mu, \mu) = \sum_{i=1}^{n} \sum_{j=1}^{n} \lambda_i \alpha_i \text{Cov}[Z_i(x_i) + Z_j(x_j), Z_i(x_i) + Z_j(x_j)] + \sigma^2 - 2 \sum_{i=1}^{n} \sum_{j=1}^{n} \lambda_i \alpha_i \text{Cov}[(Z_i(x_i) + Z_j(x_j)), Z(x)] + 2 \mu_i \left[\sum_{j=1}^{n} \lambda_j - 1\right] + 2 \mu_1 \left[\sum_{j=1}^{n} \alpha_j\right]
\]

(7)

by deriving the equation on the four variables, so that can formed the kriging weight matrix as follows:

\[
\left(\begin{array}{cccccccc}
\lambda_1 & C_{11} & \ldots & C_{1n} & C_{12} & \ldots & C_{1n}^2 & 1 & 1 \\
\lambda_2 & C_{21} & \ldots & C_{2n} & C_{21}^2 & \ldots & C_{2n}^2 & 1 & 1 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
\lambda_n & C_{n1} & \ldots & C_{nn} & C_{n2} & \ldots & C_{nn}^2 & 1 & 1 \\
\alpha_1 & C_{11}^{12} & \ldots & C_{1n}^{12} & C_{11}^{21} & \ldots & C_{1n}^{21} & 1 & 1 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
\alpha_n & C_{n1}^{12} & \ldots & C_{nn}^{12} & C_{n1}^{21} & \ldots & C_{nn}^{21} & 1 & 1 \\
\mu_1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 \\
\mu_2 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1
\end{array}\right) \left(\begin{array}{c}
C_{10}^1 \\
C_{10}^2 \\
C_{10}^3 \\
C_{10}^4 \\
C_{10}^5 \\
C_{10}^6 \\
C_{10}^7 \\
C_{10}^8 \\
C_{10}^9 \\
C_{10}^{10}
\end{array}\right)^{-1}
\]

(8)
where:

\( C_{nn} \): The variance matrix of covariance between the sampled variables at location \( n \) with the sampled variable at location \( n \).

\( C_{n0} \): The vector of covariance variance between the sampled variables at location \( n \) and the variable to be predicted.

\( \mu_1, \mu_2 \): Lagrange Multiplier Parameters.

The equation of Ordinary Co-Kriging estimator variance is as follows:

\[
\sigma^2_{ck} = \sigma^2 - \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j \text{Cov}\left[\left(Z_i(x_i) + Z_j(x_j)\right), Z(x)\right] - \mu_i.
\]

(9)

The minimum estimator variance is commonly referred to as the Ordinary Co-Kriging estimator variance, thus the best estimator satisfied the Ordinary Co-Kriging method.

2.4. Ordinary Co-Kriging Method

One of the open source software that can be used for prediction using Co-Kriging method is R software. The prediction procedure with Co-Kriging method in R software follows the following steps [14]:

1. Activation package used
The package used in the process of calculating Co-Kriging method is package GStat, package sp, package plot3D.

2. Data Input
The process of input data on the R software there is 2 ways that are, input data sets derived from the software R or input data from other files. The package that can be used to facilitate input data from another file is package Rcmdr.

3. Check the Database
After data input, the data is checked whether stationary or not. If the data is stationary and univariate it can be used Ordinary Kriging method and Simple Kriging method if the data is not stationary then it can be used Universal Kriging method, if the predicted data multivariate then can use Co-Kriging method.

4. Calculate Variogram
Calculating the Experimental Semivariogram value is required for the univariate data and calculates the Crossvariogram value for the multivariate data, as a reference for selecting the best theoretical model.

The function to calculate the value of Semivariogram and Crossvariogram by using variogram, while the function to calculate the theoretical model by using vgm.

5. Theoretical Model Fitting
Selecting the best theoretical model can be selected model based on the minimum plot of the graph and SSE. The function to choose the best model is fit.variogram.

6. Use of Lagrange Multiplier
Lagrange Multipliers are used in prediction calculations on Co-Kriging methods, to minimize prediction variance.

7. Prediction with Co-Kriging Method
The best theoretical model and Lagrange Multiplier are the inputs in the Co-Kriging method calculation, the function for calculating predictions and the minimum prediction variance using Co-Kriging method is the predict function.

3. Result and Discussion

3.1. Research Data
Based on data obtained from PT. Bumi Merapi, which is used in this research is coal quality data that is at 31 locations of drill holes with the coordinates \( x \) (meters) and \( y \) (meters). The data of coal quality can be seen in Table 1 [11].
Table 1. Coal quality data

| Lokasi | Holec | x (meter) | y (meter) | Volatile Matter (%) | Fixed Carbon (%) | Ash Content (%) | Calorific Value (cal/gr) | Total Sulphur (%) |
|---------|-------|-----------|-----------|--------------------|-----------------|-----------------|--------------------------|------------------|
| 1       | SR_01 | 350064.6  | 9579122   | 41.1               | 42.8            | 2.5             | 6340                    | 0.72             |
| 2       | SR_02 | 349636.2  | 9578921   | 40.8               | 42.5            | 3.3             | 6295                    | 0.68             |
| 30      | SR_30 | 349854.5  | 9579416   | 41                 | 42.7            | 2.1             | 6310                    | 0.61             |
| 31      | AR_30 | 350059.8  | 9578964   | 41                 | 43              | 2.1             | 6335                    | 0.6              |

(Source: PT Bumi Merapi, Lahat, South Sumatra) [11]

3.2. Correlation

The prediction process using the Ordinary Co-Kriging method, it is first to know that between the main variables and the additional variables have correlation [16]. In R 3.4.2 software and R Studio 1. 1.383 to calculate the correlation value between each variable with other variables can use the function `corr(variable1, variable2)` so that it can be seen the correlation value of the variables in Table 2.

Table 2. Correlation between coal quality variables

| Correlation          | Volatile Matter (%) | Fixed Carbon (%) | Ash Content (%) | Calorific Value (cal/gr) | Total Sulphur (%) |
|----------------------|---------------------|------------------|-----------------|--------------------------|------------------|
| Volatile Matter (%)  | 0                   | 0.573501         | -0.67357        | 0.678446                 | 0.236576         |
| Fixed Carbon (%)     | 0.573501            | 0                | -0.60292        | 0.55653                  | -0.08583         |
| Ash Content (%)      | -0.67357            | -0.60292         | 0               | -0.49344                 | 0.008083         |
| Calorific Value (cal/gr) | 0.678446         | 0.55653          | -0.49344        | 0                        | 0.151062         |
| Total Sulphur (%)    | 0.236576            | -0.08583         | 0.008083        | 0.151062                 | 0                |

From the output results in Table 2 obtained correlation coefficient between variables of coal quality which states the level of closeness between variables. Based on the Guilford classification, the correlation values can be classified based on the coefficient interval [17]. The correlation coefficient values in Table 2 and referring to the Guilford Table can be selected from all correlation values between the coal quality variables that are used for prediction calculations by the Ordinary Co-Kriging method are the correlation coefficients that are in the coefficient intervals of 0.4000 - 0.599 or medium, and coefficient intervals of 0.600 - 0.799 or high/strong. From the result of output obtained that there is three correlation coefficient that fulfills the criteria, that is the coefficient correlation of Volatile Matter and Fixed Carbon equal to 0.573501, Volatile Matter and Calorific Value correlation coefficient equal to 0.678446, and Fixed Carbon and Calorific Value correlation coefficient 0.55653. The most influential factor on the quality of coal is the content of Fixed Carbon and Calorific Value greatly affect the coal combustion process to produce Fixed Carbon according to the criteria. So in this study used variable Fixed Carbon and Calorific Value for calculation with Co-Kriging method.

3.3. Crossvariogram Fixed Carbon and Calorific Value

The cross-variogram value is calculated on the basis of all possible distance pairs where the distance function used is the Euclidean distance, the function of distance $h$ which expresses the difference of the main variable by the difference of the additional variables spaced $h$, using equation (1) can be obtained the cross-variogram value along with the number distance pair. The sampled research data consisted of 31 borehole locations so as to make the calculation process manually for cross variogram value of Fixed
Carbon and Calorific Value to be difficult. Required software assistance to facilitate the process of calculating the cross-variogram value, in the software R 3.4.2 and R Studio 1.1.383 to calculate the cross-variogram value can use variogram and v.cross functions so that the calculation of cross-variogram values for Fixed Carbon and Calorific Value in Table 3.

Table 3. Crossvariogram fixed carbon and calorific value

| Number of point pairs with same distance | Crossvariogram Fixed Carbon and Calorific Value |
|----------------------------------------|-----------------------------------------------|
| 1                                      | 2                                             |
| 2                                      | 158.2518                                      |
| 3                                      | 162.8169                                      |
| 4                                      | 272.7568                                      |
| 5                                      | 346.7899                                      |
| 6                                      | 442.9263                                      |
| 7                                      | 523.3112                                      |
| 8                                      | 597.8671                                      |
|                                        | 667.4127                                      |

Based on Table 3 shows that from 31 locations sampled there are 8 criteria of the number of pairs of data that are equidistant, and can be seen that there are 32 most data pairs that have a distance of 523.3112, it means that most of the locations of the samples are spread that spread at the location of the drill hole has a distance with a cross-variogram of 24.9062. The plot is obtained in Figure 1 of the cross-pathogram value to the distance \((h)\) where all information is synthesized in a point per distance class, which then plots are used for the best theoretical model fitting.

![Figure 1. Plot of crossvariogram fixed carbon and calorific value](image)

3.4. Theoretical Model Fitting for Fixed Carbon and Calorific Value

The process of cross-variogram fitting with theoretical model approach can be done in two stages:
1. Perform the process of calculating theoretical models on the three models used, then made plot and can be visible visually based on the plot of the fitting.
2. Specified based on the minimum SSE of the three models.

After the theoretical model calculation is done, then fitting between cross-variogram with the theoretical model using the function `fit.variogram` then plotted and can be seen in Figure 2.
According to Figure 2, it can be seen from the three approaches of the theoretical model that best match the cross-variogram between Fixed Carbon and Calorific Value is the Gaussian model, for more accurate results calculated SSE (Sum Square Error) of the three models and can be seen in Table 4.

**Table 4. SSE crossvariogram fixed carbon and calorific value**

| Model     | Exponential | Gaussian | Spherical |
|-----------|-------------|----------|-----------|
| SSE       | 0.1442817   | **0.1005384** | 0.1129344 |

Based on Table 4 of the three theoretical models obtained the Gaussian model which has the minimum SSE of 0.1005384, so the Gaussian model is used as input in the calculation process of the Co-Kriging method.

### 3.5. Prediction of Co-Kriging Method for Fixed Carbon and Calorific Value

Having obtained the Gaussian model from the fitting result, the model is used as input in Co-Kriging method. The objective of Co-Kriging method is to predict in unobserved locations, based on the research data that were sampled as many as 31 locations of drill holes were predicted at 30 unobserved locations around the dotted locations. Prediction is calculated by using Software R 3.4.2 and R Studio 1.1.383 by using predict function. The prediction and prediction variance can be seen in Table 5.
Table 5. Prediction fixed carbon and calorific value at unobserved locations

| Loc | Coordinates         | Prediction Fixed Carbon (%) | Prediction Variance FC | Prediction Calorific Value (cal/gr) | Prediction Variance CV | Covariance FC and CV |
|-----|---------------------|-----------------------------|------------------------|-----------------------------------|------------------------|-----------------------|
| 1   | (349425, 9579763)   | 43.42679                    | 27.45485               | 6350.501                          | 6967.063               | 1.150461              |
| 2   | (349212, 9578992)   | 43.47533                    | 27.45826               | 6337.611                          | 7207.823               | 0.243748              |
| 3   | (349468, 9579543)   | 43.46146                    | 27.44951               | 6341.296                          | 6590.501               | 2.568616              |
| ... |                     | ...                         | ...                    | ...                               | ...                    | ...                   |
| 28  | (346102, 9579485)   | 43.4373                     | 27.44377               | 6347.71                           | 6186.053               | 0.4551792             |
| 29  | (348420, 9578789)   | 43.44905                    | 27.45801               | 6344.59                           | 7189.814               | 0.4551792             |
| 30  | (346168, 9579856)   | 43.25528                    | 27.44201               | 6396.041                          | 6061.664               | 0.4551792             |

Based on Table 5, the predicted results at unobserved locations, the prediction variables of each variable, and the prediction covariance of Fixed Carbon and Calorific Value by using Ordinary Co-Kriging method, then can be seen the summary of the predicted results in Table 6 to measure the accuracy of predicted results.

Table 6. Summary of prediction fixed carbon and calorific value results

| Prediction Fixed Carbon (%) | Prediction Variance FC | Prediction Calorific Value (cal/gr) | Prediction Variance CV | Covariance FC and CV |
|-----------------------------|------------------------|------------------------------------|------------------------|-----------------------|
| Minimum                     | 43.2                   | 27.39                              | 6200                   | 2498                  | -0.3173               |
| 1st Quartil                 | 43.43                  | 27.44                              | 6337                   | 6062                  | 0.3516                |
| Median                      | 43.46                  | 27.45                              | 6342                   | 6551                  | 2.7177                |
| Mean                        | 43.46                  | 27.45                              | 6341                   | 6336                  | 3.5255                |
| 3rd Quartil                 | 43.48                  | 27.46                              | 6351                   | 7179                  | 4.5605                |
| Maximum                     | 44                     | 27.46                              | 6410                   | 7357                  | 17.9806               |

Based on Table 6 it is found that the average Fixed Carbon prediction result is 43.46% which means the same with the average of the sample data is 43.46%, the minimum value of the predicted result is 43.2% which means quite close to the minimum value of the sample data of 42.30% the maximum value of the predicted result of 44% which means quite close to the maximum value of the sample data of 44.50%. As for Calorific Value, the average predicted result is 6341 cal/gr, which means close to the average of the sample data of 6340 cal/gr, the minimum value of the predicted result is 6200 cal/gr which means it is close to the minimum value of the sample data 6000 cal/gr, the maximum value of the predicted results of 6410 which means close to the maximum value of the sample data of 6455. It can be concluded that the prediction of the predicted results close to the calculation of sample data, so that Co-Kriging method is used to predict Fixed Carbon content influenced by variable Calorific Value.

4. Conclusion
The Lagrange Multiplier Approach to the Kriging method is used to derive the predicted variance equation of the Ordinary Co-Kriging estimators of two complete variables, to produce the minimum estimator variance. In this research, we developed the procedure of using Lagrange Multiplier to get the minimum prediction variance after prediction result obtained. The process of calculating the prediction
of coal quality by using the functions in R 3.4.2 software and R Studio 1.1.383 for Ordinary Co-Kriging method on variable Fixed Carbon and Calorific Value produce the best theoretical model is Gaussian model as input in the prediction calculation at unobserved locations. The result of the Lagrange Multiplier approach on Ordinary Co-Kriging method using R software produces faster, precise, and accurate calculations.

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