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Research Paper

A simulation comparison of ordinary kriging with indicator kriging

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Abstract: Spatial data analysis methods have many applications in various fields, such as agriculture, mining engineering, and meteorology. In this study, ordinary kriging and indicator kriging are considered to predict alumina grade in the Jajarm mine in Iran, and the precision of the methods is computed. A conditional simulation is carried out based on the data set for a more general comparison of ordinary and indicator kriging to interpolate Alumina grade in the mine. In the case of monitoring possible variation related to sample size and type of variogram model, simulations are performed with various sample sizes and different types of variogram models. Then ordinary and indicator kriging methods are applied for every set of simulated data (concerning different sample sizes and types of variogram models), and root of standardized mean square error prediction is considered as a cross-validation criterion to compare the kriging methods. The simulation results show that under the assumptions, ordinary kriging has better performance than the indicator kriging method.

Keywords: Cross-validation; Indicator kriging; Ordinary kriging; Random field; Root of standardized mean squared errors prediction; Spatial data.
Mathematics Subject Classification (2010): 62P99.

1 Introduction

Kriging method was first introduced by Daniel Krige that used it to predict ore grades in the gold mines of south Africa (Krige, 1951, 1966). The empirical approach of Krige was formalized by Matheron (1963) and the term "kriging" was coined in his honor. In

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the following two decades, lots of environmental scientists used kriging in their fields (Burgess and Webster, 1980; DeMarsily and Ahmed, 1987; Oliver and Webster, 1987; Munyati and Sinthumule, 2021).

To estimate the values at unsampled locations, kriging uses nearby samples and calculates their weighted average. But first, one needs to estimate the variogram function, which shows the correlations among neighboring values as a function of distance between the points across the study area.

This research aims to compare two spatial interpolation techniques based on the kriging theory. The kriging techniques, ordinary kriging, and indicator kriging have been applied to interpolate grades of alumina in the Jajarm bauxite mine in Iran.

Additionally, a simulation study is carried out based on the Jajarm data set. Different sample sizes and different variogram models are used to monitor their influence over the interpolation results. The performance of the methods is assessed by a criterion of cross-validation, namely the root of standardizedm Mean squared errors prediction (RSMP). The results of the simulation imply that regardless of the sample size and the type of variogram model used, ordinary kriging has better performance than indicator kriging.

In section 2, the kriging methods are discussed. The variogram plays a crucial role in these methods. Section 3 discusses some aspects of the variogram. In section 4, the kriging methods are applied to predict the grade of alumina for the Jajarm data set. In this process, different variogram models are fitted to the empirical variogram of the data, and the performance of the kriging methods is computed in each case.

Furthermore, to determine the more efficient kriging method for predicting the grade of alumina in the Jajarm mine, a simulation study is performed based on the data set, and the performance of the kriging methods is compared.

2 Kriging

Kriging methods are applied to provide optimal predictions of unobserved values in a random field. In this section, ordinary kriging and indicator kriging methods are reviewed.

2.1 Ordinary kriging

Spatial data refers to data that is associated with a specific geographic location or coordinate on the earth's surface. In spatial data analysis, a random field is defined as $\{Z(s); \quad s \in D\}$ where $D \in \mathbb{R}^d$, and $Z(s)$ is a random variable in position s.

Ordinary kriging does not require the mean (μ) of the random field $Z(s)$ to be known, being evaluated from the input data.

If the random field $Z(.)$ is intrinsically stationary, with an unknown mean, ordinary kriging is the suitable estimation method. The random field for ordinary kriging can be represented by the model:

$$Z(s) = \mu + e(s), \qquad s \in D, \tag{1}$$

where μ is the mean of the process and $e(.)$ is a random quantity that its mean is zero and its covariogram equals $C(h)$, where h is the separation in space and is known as

the lag. Then, predictions at new locations are made by:

$$\hat{Z}(s_0) = \sum_{i=1}^{n} l_i Z(s_i); \qquad \sum l_i = 1,$$

where l_is are the weights calculated by the related variogram model and n is the sample size.

Now, the method of computing kriging weights (l_is) is explained: Kriging provides optimal predictors. Optimal predictor refers to the case of squared-error loss and hence of minimizing mean-squared prediction error, Therefore, the optimal $\hat{Z}$ minimizes the mean-squared prediction error

$$\sigma_e^2 = E(Z(.) - \hat{Z}(.))^2, \tag{2}$$

over the class of linear predictors $\sum_{i=1}^{n} l_i Z(s_i)$ that satisfy $\sum_{i=1}^{n} l_i = 1$.

For ordinary kriging, the minimization of relation (2) is carried out over $l_1, l_2, \ldots, l_n$, subject to $\sum_{i=1}^{n} l_i = 1$, where the model (1) is assumed to hold with variogram

$$2\gamma(h) = var(Z(s+h) - Z(s)), \qquad h \in \mathbb{R}^d.$$

Therefore to minimize equation (2) with Lagrange method, the follwing equation should be minimized

$$E(Z(s_0) - \sum_{i=1}^{n} l_i Z(s_i))^2 - m(\sum l_i - 1), \tag{3}$$

with respect to $l_1, \ldots, l_n$ and Lagrenge multiplier, m.

From (3) it can be shown that the optimal $l_1, l_2, \ldots, l_n$ can be obtained from

$$\boldsymbol{L}_0 = \Gamma_0 \boldsymbol{\gamma}_0,$$

where $\boldsymbol{L}_0 = (l_1, l_2, \ldots, l_n, m)'$, $\gamma_0 = (\gamma(s_0 - s_1), \ldots \gamma(s_0 - s_n), 1)'$ and

$$\Gamma_0 = \begin{cases} \gamma(s_i - s_j), & i = 1, 2, \ldots, n, j = 1, 2, \ldots, n, \\ 1, & i = n+1, j = 1, 2, \ldots, n, \\ 0, & i = n+1, J = n+1. \end{cases}$$

Γ_0 is a symmetric matrix of dimension $n+1$. These weights are used in the computation of ordinary kriging. For further details, please refer to Cressie (1993).

2.2 Indicator kriging

Indicator kriging is a non-parametric geostatistical method that works with variables after indicator transformation (0, 1) of pre-defined threshold values and maps the probability of exceeding pre-defined threshold values. Therefore, unlike other kriging methods, it is not necessary to have information about the distribution of observations. Sometimes the actual values of the variable are not important, but the probability of the variable exceeding a certain threshold is considered. For example, to obtain the probability of pollution of an area exceeding the standard level or to determine the

probability of the grade of a mineral exceeding a certain value (in order to check the economic feasibility of starting exploration operations), indicator kriging is used.

To estimate the probability of the variable value exceeding a certain threshold, the indicator kriging method is used. This threshold is considered for the variable alumina 40. (The mining expert determines the value of threshold 40 in the Jajarm mine dataset). In this research, kriging calculates the probability of the alumina metal grade exceeding 40 in places without samples (in other words, the places where the alumina metal grade is more than 40 with a significant probability are identified).

The model of indicator kriging could be written as

$$I(s) = \mu + e(s),$$

where μ is an unknown constant and $I(s)$ is a binary variable. The creation of binary data may be through the use of a threshold for continuous data, or it may be that the observed data is 0 or 1 (Hohn, 1998). In the other words, the indicator random variables

$$I(s_0, z) = \begin{cases} 1, & Z(s_0) \leq z, \\ 0, & otherwise, \end{cases}$$

is considered, where $s \in D, z \in \mathbb{R}$.

It can be shown easily that $E(I(s_0, z)) = Pr(Z(s_0) \leq z)$. The indicator predictor of $I(s_0, z)$ based on data $(I(s_1, z), \ldots, I(s_n, z))$ is

$$\hat{I}(s_0, z) = \sum_{i=1}^{n} l_i(z) I(s_i, z),$$

where $\sum_{i=1}^{n} l_i(z) = 1$, and $l_i(z)$'s satisfy

$$\sum_{i=1}^{n} l_i(z)\gamma(s_i - s_j) + m = \gamma(s_0 - s_j), \quad j = 1, \ldots, n, z \in \mathbb{R},$$

where m is the Lagrange multiplier and γ is the semivariogram. The weights, $l_i(z)$s may be obtained as the mentioned manner explained for ordinary kriging earlier in this section (Cressie (1993)).

2.3 Variogram

Assuming that $Z(.)$ is intrinsically stationary, it can easily be shown that variogram is $2\gamma(h) = E((Z(s+h) - Z(s))^2)$ and $\gamma(h)$ is called Semivariogram. Empirical variograms are nonparametric estimators of the variogram $2\gamma(h)$, is

$$2\hat{\gamma}(h) = \frac{1}{|N(h)|} \sum_{N(h)} [Z(s_i) - Z(s_j)]^2,$$

where $N(h) = \{(s_i, s_j) : s_i - s_j = h;\ i, j = 1, 2, \ldots, n\}$ and $|N(h)|$ denotes the number of unique pairs of locations in $N(h)$. When $Z(.)$ is isotropic, the empirical variogram can be written as a function of the distance between pairs of observations. In this case, a powerful graphical tool for exploring the spatial dependence structure of $Z(.)$ is a scatter plot of the empirical variogram, $2\hat{\gamma}_h$ against $||h||$ (Calder and Cressie (2009)).

2.3.1 Variogram models

In this section, some variogram models are reviewed. Besides, plots of fitting the variogram models (solid lines) to empirical semivariogram (dots) for the Jajam mine dataset are given.

Spherical semivariogram

spherical semivariogram is defined as

$$\gamma(h) = \begin{cases} c(\frac{3h}{2a} - \frac{1}{2}(\frac{h}{a})^3), & h \leq a, \\ c, & h > a, \end{cases}$$

where a is the range, r is the spatial extent parameter and c is the sill.

Exponential model

The model is given by $\gamma(h) = c(1 - \exp(\frac{-h}{r}))$, where a is the range, and parameter r defines the spatial extent of the model. Figure 1 illustrates the fitting of exponential semivariogram (plot a), and spherical semivariogram (plot b), to the empirical semivariogram [dots] of alumina in the Jajarm dataset.

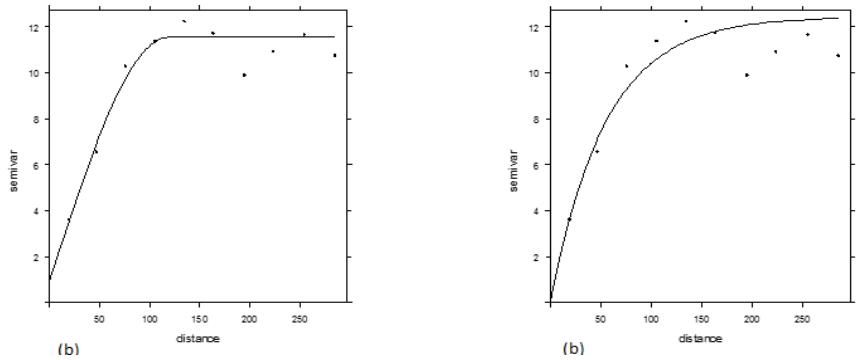

Figure 1: plot (a): Exponential semivariogram; plot (b): Spherical semivariogram.

Circular semivariogram

The formula for the circular semivariogram is

$$\gamma(h) = \begin{cases} c(1 - \frac{2}{\Pi} cos^{-1}(\frac{h}{a}) + \frac{2h}{\Pi a}\sqrt{1 - \frac{h^2}{a^2}}), & h \leq a, \\ c, & h > a, \end{cases}$$

where c and a are the sill and the range.

Gaussian model

Gaussia semivariogram is defined as $\gamma(h) = c(1 - \exp(\frac{-h^2}{r^2}))$, where c is the sill, h is the lag distance, and r is the spatial extent parameter. Figure 2 indicates Circular model (plot c), and Gaussian model (plot d) as solid line and the empirical semivariogram is denoted by dots.

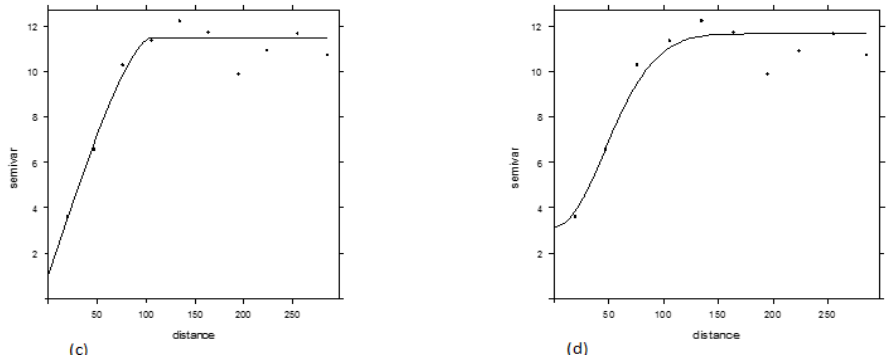

Figure 2: plot (c): Circular semivariogram, plot (d): Gaussian semivariogram.

Wave semivariogram

A semivariogram model that exhibits nagative correlations caused by a periodicity of the process is the wave (or hole-effect) model:$\gamma(h) = c[1 - \frac{\sin(h)}{h}]$, where c is the sill and h is the lag distance. Figure 3 shows the fitted wave semivariogram (as the contunoius line) to the empirical variogram as dots, based on Jajarm mine dataset. For more details on variogram models, please refer to Wester and Oliver (2007).

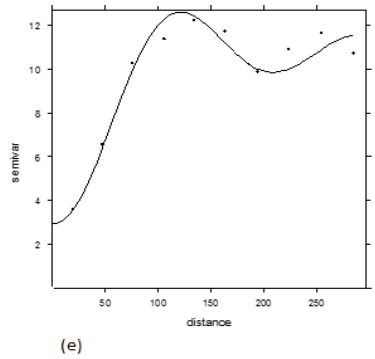

Figure 3: Wave semivariogram as solid line and empirical semivariogram as dots.

2.4 Cross-validation

To compare the method's performances, a criterion should be considered. Cross-validation is a popular means of assessing statistical estimation and prediction. If the variogram model described adequately spatial dependencies implicit in a data set,

then the predicted value $\hat{Z}(t_0)$ should be close to the true value $Z(t_0)$. Ideally additional observations on $Z(.)$ to check this, or initially some of the data might be set aside to validate spatial predictor. More likely, all of the data are used to fit the variogram, build the spatial predictor and there is no possibility of taking more observations. In this case, the cross-validation approach can be used. Let $2\hat{\gamma}(h)$ be the fitted variogram model (obtained from the data); now delete a datum $Z(t_j)$ and predict it with $\hat{Z}_{-j}(t_j)$ [based on $2\hat{\gamma}(h)$ variogram estimate and the data without $Z(t_j)$].

The closeness of prediction values to the true values can be characterized as cross-validation criteria. the Root of Standardized Mean Squares Error Prediction (RSMP) is a cross-validation criterion

$$RSMP = [\frac{1}{n}\sum_{i=1}^{n}(\frac{Z(t_j) - \hat{Z}_{-j}(t_j)}{\sigma_{-j}(t_j)})^2]^{1/2},$$

where $\hat{Z}_{-j}(t_j)$ is the predict of true value $Z(t_j)$ after deleting j'th datum, $\sigma^2_{-j}(t_j)$ is the related standard deviation, and n is the number of observations. For more details, please refer to Cressie (1993).

In this study, RSMP criterion is applied to compare ordinary and indicator kriging methods.

3 Comparison of ordinary kriging with indicator kriging

In this section, the real data set of alumina in the Jajarm mine (in Iran) is considered. The mine is located 175 km from Jajarm city in South Khorasan province. In Figure 4, sample points in the dataset are shown in the Jajam Bauxite mine.

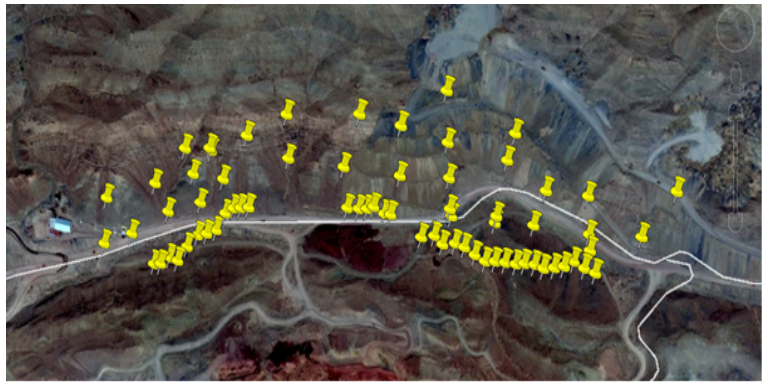

Figure 4: Scattering of sample points in the Jajam Bauxite mine.

To utilize kriging methods, it is imperative to satisfy two conditions: stationarity and the Gaussian distribution of the data. The exploratory studies demonstrate these conditions are satisfied for the Jajarm dataset. The means of stationarity here is the

absence of a trend in both directions. Plot 5 shows that there is no trend in the two directions.

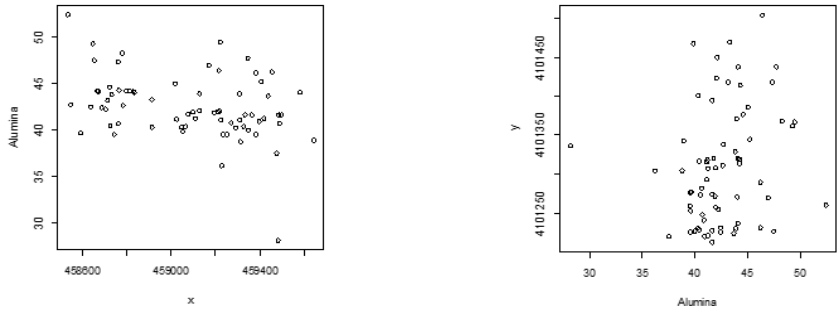

Figure 5: Scatterplot of alumina with respect to the x-axis (left) and respect to the y-axis (right).

In Table 1, ordinary and indicator kriging methods are compared for the data set.

Table 1: RSMP of alumina in ordinary and indicator kriging.

	Spherical	Exponential	Circular	Gaussian	Wave
Ordinary Kriging	0.97	0.98	0.96	0.97	1.01
Indicator Kriging	0.88	0.90	0.86	0.88	0.92

Table 1 shows that the circular variogram has the best performance for this data set in ordinary and indicator kriging methods. Besides, for this data set, the RSMP of indicator kriging is smaller than ordinary kriging.

Prediction map and prediction variance map of alumina grade in the mine are obtained by using ordinary kring and are shown in Figure 6.

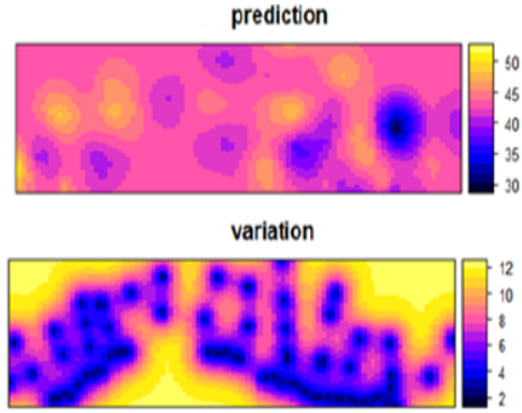

Figure 6: Prediction map (above) and prediction variance map (below).

To investigate a more precise comparison of ordinary and indicator kriging methods to predict alumina grade in the mine, conditional simulation based on the data is considered, and the simulation results are presented in the following. In the simulation

study, the effects of different sample sizes and different types of variograms are assessed. The results have been presented in Table 2.

Table 2: RSMP of kriging methods based on variogram.

Variogram	n	Ordinary kriging	Indicator kriging
Circular	49	0.90	0.88
	100	0.72	0.76
	225	0.62	0.82
	400	0.55	0.76
Spherical	49	0.92	0.88
	100	0.73	0.76
	225	0.64	0.82
	400	0.62	0.78
Exponential	49	0.96	0.88
	100	0.72	0.70
	225	0.64	0.70
	400	0.54	0.66
Gaussian	49	0.94	0.90
	100	0.71	0.78
	225	0.61	0.82
	400	0.56	0.76
Wave	49	0.90	0.94
	100	0.66	0.80
	225	0.76	0.82
	400	0.56	0.80

Table 2 shows that for the simulated data based on the circular variogram, errors that are assigned to indicator kriging in all sample sizes are larger than ordinary kriging. Therefore, ordinary kring based on the circular variogram has better performance than the indicator kriging method. Also, ordinary kriging's errors in the most of sample sizes based on the spherical variogram are smaller than the other method. Then, applying ordinary kriging is preferred. As indicated for simulated data based on exponential variogram, ordinary kriging for simulated data has better performance than indicator kriging for every sample size except sample size 49. The simulated data based on the Gaussian variogram demonstrates the error values that are assigned to ordinary kriging in most of the sample sizes are smaller than the other kriging method. In addition based on the wave variogram, errors that are assigned to ordinary kriging are smaller than indicator kriging. Therefore, ordinary kring based on wave variogram has better performance than indicator kriging.

Finally, the simulation results show that ordinary kriging has better performance than indicator kriging for the most of sample sizes and every considered variogram. Then, to predict the alumina grade in the Jajarm mine for unsampled points, the application of ordinary kriging is preferred.

4 Discussion and conclusions

Kriging methods are applied to predict attribute values at unsampled locations in spatial data. These methods have numerous applications in the environmental sciences. In this article, two kriging methods, namely ordinary kriging and indicator kriging, are used to predict the alumina grade in an Iranian mine.

The variogram model plays an important role in kriging methods. Therefore, to determine the best variogram model, the empirical variogram of the data is calculated and various variogram models are fitted to it. The results show that the circular model of the variogram performs best for both ordinary and indicator kriging methods. To ensure a more accurate comparison between ordinary kriging and indicator kriging in the mine, a conditional simulation is performed based on the dataset. In the simulation study, various variogram models and sample sizes are evaluated to investigate the effect of sample size and the variogram model. The RSMP is used as a cross-validation criterion to compare the methods. The results of the simulation study show that regardless of the dataset size and variogram models used, ordinary kriging outperforms the alternative kriging method. Therefore, it is recommended to use ordinary kriging for predicting the alumina grade in the mine.

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