Linearity and Lagrange Linear Multiplicator in the Equations of Ordinary Kriging

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The equations of Simple and Ordinary Kriging are compared to outline their differences in the estimation procedure. Emphasis is given to the Lagrange multiplicator as a variable that allows the minimization of variance in Ordinary Kriging. The matrices and linear systems of kriging, which are most often performed in the background of the computer mapping algorithm, are analyzed and presented in detail. The intention is to show the importance of geomathematics in one of the basic geological tasks, mapping. Furthermore, a detailed presentation of equation sets provides a better understanding of the Simple and Ordinary Kriging algorithms for geological engineers, as the two most-used geostatistical techniques (included Indicator Kriging as the third). The conclusion includes proposals, presented in four steps, for the determination of the Lagrange multiplicator value in any Ordinary Kriging equation.

Key words: geostatistics, kriging, linear estimator, Lagrange multiplier

1. INTRODUCTION

The kriging method is considered a progressive interpolation method for the estimation of a regionalized variable at selected grid points. The term *regionalized variable* refers to such variables, which can be regarded to be random variable in the infinitely small surrounding of a particular location, but there exist a function above the region which can relate these variables to each other. The term "random" assumes that the probability of the variable being smaller than a real number exists for any real number.

Kriging, as a statistical estimation method, is named after South Afrikaans engineer Krige[6], who first applied and described this methodology to estimate gold concentrations in ore deposits. This was followed by further theoretical development of the method, predominantly by French scientists, especially Matheron[11]. Finally, several kriging techniques have been defined with different equations (such as Simple, Ordinary, and Indicator Kriging, and others).

Kriging estimation is based on the application of existing measurements (so-called "control points"), whose influence on the estimation is expressed with weighting coefficients. This estimation also assumes the satisfaction of the relevant criteria. This means that the estimation must be unbiased and performed so that the variance between the measured and estimated values at the selected points is as low as possible. Such a value is also called the "kriging variance", which represents the interpolation quality and can be compared with a cross-validation technique.

In every kriging techniques, the procedure for minimizing the estimation error includes a variable called the "Lagrange multiplicator". The purpose of the analysis presented here is to describe the mathematical meaning of the multiplicator and its role in minimizing the kriging variance.

2. KRIGING PROPERTIES

Kriging techniques belong to a set of linear algorithms that are based on the least squares method. The selection of the appropriate technique is based on the properties of the random variable that is to be interpolated by kriging. The techniques are based on the estimation of weighting coefficients with an assumption of unbiasedness. Each hard data has its own weighting coefficient (λ), which represents the influence of a particular data on the value of the final estimation at the selected grid node. The relationship between the existing (hard) data and the estimation point has been expressed by variogram values (if we suppose the existence of intrinsic hypothesis) or by covariance in case of second order stationarity. Such values describe the spatial dependence and the influence of the particular location in terms of its distance and direction from the estimated location (point).

A spatial model based on a larger number of control points, a higher variogram range, a lower nugget effect, and without anisotropy is usually much more reliable. Regardless of the spatial dependence described by the variogram or the covariance function, the weighting coefficient at a particular location is exclusively a measure of the distance and orientation between data points. This means that the measurement values at the observed points do not influence the variogram or the covariance values. Higher variogram values (within the range of influence) indicate an increasing "order" or estimation reliability, i.e., higher values for any pair of points indicate a greater interaction between those locations supposing that their separation distance smaller than the range of influence. An additional estimation quality can be reached by the regular distribution of the control points. Because of all its advantages as a statistical interpolation technique, kriging is described as the "best linear unbiased estimator" or by the acronym "BLUE".

In the text below, the detailed meaning of linearity in Simple and Ordinary Kriging, and how such linearity is achieved, will be described.

3. MATHEMATICAL FUNDAMENTALS OF KRIGING

The principle of kriging is shown most simply with sets of equations that define the method. Kriging is applied to the estimation of the values of a regionalized variable at a selected location (Z_k), based on surrounding existing values (Z_i). Each such location is assigned a relevant weighting coefficient (λ_i), and the calculation of this is the most demanding part of the kriging algorithm. The value of a regionalized variable can be defined as:

$$Z_i = Z(x_i) \tag{3.1}$$

where

x_i is the value at the known location.

Moreover, the value of a regionalized variable estimated by kriging based on n points is:

$$Z_k = \sum_{i=1}^{n} \lambda_i \cdot Z_i \tag{3.2}$$

where

λ_i is the weighting coefficient for a particular location "i";

Z_i are known values, the so-called "control points" (hard data);

Z_k is the value estimated by kriging.

These equations represent the system of linear kriging equations that is described in numerous books, e.g., references[3, 4, 5, 7] and others.

Equation 3.2 can be written as the matrix Equation 3.3. In both of these matrices, the values are expressed as variogram values, i.e., these values depend only on the distances and orientations between the control points and not on their values. The third matrix includes weighting coefficients, which are simply estimated from a system with "n" equations with "n" unknown variables.

$$[A]\cdot[\lambda] = [B] \tag{3.3}$$

The method of kriging includes several techniques. These are Simple Kriging, Ordinary Kriging, Indicator Kriging, Multiple Indicator Kriging, Universal Kriging, IRFk Kriging, Lognormal Kriging, and Disjunctive Kriging. In the following comparison of simple and ordinary kriging, we will describe the effect caused by including of the linear coefficient in the kriging equations to achieve unbiasedness.

3.1. Simple Kriging theory

Simple kriging, as its name implies, is the simplest kriging technique. The full matrix equation is:

$$\begin{bmatrix} \gamma(Z_1-Z_1) & \gamma(Z_1-Z_2) & \dots & \gamma(Z_1-Z_n) \\ \gamma(Z_2-Z_1) & \gamma(Z_2-Z_2) & \dots & \gamma(Z_2-Z_n) \\ & & & \\ \gamma(Z_n-Z_1) & \gamma(Z_n-Z_2) & \dots & \gamma(Z_n-Z_n) \end{bmatrix} \cdot \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \\ \lambda_n \end{bmatrix} = \begin{bmatrix} \gamma(Z_1-Z) \\ \gamma(Z_2-Z) \\ \\ \gamma(Z_n-Z) \end{bmatrix} \tag{3.4}$$

where

γ are the variogram values;

$Z_1 \dots Z_n$ are known measured values at points;

Z is the point at which new values are estimated from known (hard) data ($Z_1 \dots Z_n$).

Kriging uses dimensionless point data that represent the values of the regionalized variable. In Simple Kriging, it is assumed that the regionalized variable has second order stationary, the excepted value is everywhere constant and known $[\mu(x) = 0]$, and the covariance function is known $[c(x, y) = Cov(Z(x), Z(y))]$. Furthermore, when this estimation is performed at the control point, the error can also be calculated at the point as:

$$\varepsilon = (Z_{real} - Z_{estimated}) \tag{3.5}$$

If there is no external drift in the variable and the sum of all weighting coefficients is 1, unbiasedness is achieved. The difference between all the measured and estimated values is called the **estimation error** or **kriging variance** and it is expressed as:

$$\sigma^2 = \frac{\sum_{i=1}^{n} (Z_{real} - Z_{estimated})_i^2}{n} \tag{3.6}$$

It can also be shown as the second square of the variance or the **standard error** of the estimation:

$$\sigma = \sqrt{\sigma^2} \tag{3.7}$$

In an ideal case, kriging tries to calculate the optimal weighting coefficients that will lead to the minimal estimation error. Such coefficients, which lead to an estimation of unbiasedness with minimal variance, are calculated by solving of the matrix equations system. If the matrices in Equation 3.4 is represented by linear equations, it can be written as:

$$\begin{aligned} &\gamma(Z_1-Z_1)\cdot\lambda_1 + \gamma(Z_1-Z_2)\cdot\lambda_2 + \dots + \gamma(Z_1-Z_n)\cdot\lambda_n = \gamma(Z_1-Z) \\ &\gamma(Z_2-Z_1)\cdot\lambda_1 + \gamma(Z_2-Z_2)\cdot\lambda_2 + \dots + \gamma(Z_2-Z_n)\cdot\lambda_n = \gamma(Z_2-Z) \\ &\dots\dots \\ &\gamma(Z_n-Z_1)\cdot\lambda_1 + \gamma(Z_n-Z_2)\cdot\lambda_2 + \dots + \gamma(Z_n-Z_n)\cdot\lambda_n = \gamma(Z_n-Z) \end{aligned} \tag{3.8}$$

The estimation is the selected point that can be represented by the following equation:

$$Z = \frac{\begin{pmatrix} \lambda_1 \\ \\ \lambda_n \end{pmatrix} \cdot \begin{pmatrix} \gamma(Z_1-Z_0) \\ \dots \\ \gamma(Z_n-Z_0) \end{pmatrix}}{\begin{pmatrix} \gamma(Z_1-Z_1) & \dots & \gamma(Z_1-Z_n) \\ \dots & \dots & \dots \\ \gamma(Z_n-Z_1) & \dots & \gamma(Z_n-Z_n) \end{pmatrix}} \tag{3.9}$$

Moreover, for Equation 3.8 to be considered unbiased, an additional condition must be fulfilled, i.e., the sum of all weighting coefficients is 1 ($\sum_{i=1}^{n} \lambda_i = 1$). This condition is achieved by adding new conditions to the kriging matrices like Lagrange multiplicator in Ordinary Kriging equations.

3.2. Ordinary kriging theory

All others kriging techniques add some constraints to the matrices, to minimize the error $\sigma_k^2(x)$, and these techniques are unbiasedness estimations. Generally, these factors would describe some external limit (restriction) on the input data, which cannot simply be observed in the measured values. The most-used kriging technique is probably ordinary kriging, and we therefore analyse the constraint factor in Ordinary Kriging equations, called the *Lagrange multiplicator*.

As discussed above, if the sum of all weighting coefficient is 1, Expression 3.8 can be written as:

$$\begin{aligned}
&\gamma(Z_1-Z_1)\cdot\lambda_1+\gamma(Z_1-Z_2)\cdot\lambda_2+\ldots+\gamma(Z_1-Z_n)\cdot\lambda_n+m=\gamma(Z_1-Z)\\
&\gamma(Z_2-Z_1)\cdot\lambda_1+\gamma(Z_2-Z_2)\cdot\lambda_2+\ldots+\gamma(Z_2-Z_n)\cdot\lambda_n+m=\gamma(Z_2-Z)\\
&\ldots\ldots\\
&\gamma(Z_n-Z_1)\cdot\lambda_1+\gamma(Z_n-Z_2)\cdot\lambda_2+\ldots+\gamma(Z_n-Z_n)\cdot\lambda_n+m=\gamma(Z_n-Z)\\
&\lambda_1+\lambda_2+\ldots+\lambda_n+0=1
\end{aligned} \tag{3.10}$$

If such a system of linear equations is shown as a matrices it can be written as:

$$\begin{bmatrix}
\gamma(Z_1-Z_1) & \gamma(Z_1-Z_2) & \ldots & \gamma(Z_1-Z_n) & 1\\
\gamma(Z_2-Z_1) & \gamma(Z_2-Z_2) & \ldots & \gamma(Z_2-Z_n) & 1\\
\ldots & & & & \\
\gamma(Z_n-Z_1) & \gamma(Z_n-Z_2) & \ldots & \gamma(Z_n-Z_n) & 1\\
1 & 1 & \ldots & 1 & 0
\end{bmatrix}\cdot\begin{bmatrix}\lambda_1\\ \lambda_2\\ \\ \lambda_n\\ m\end{bmatrix}=\begin{bmatrix}\gamma(Z_1-Z)\\ \gamma(Z_2-Z)\\ \\ \gamma(Z_n-Z)\\ 1\end{bmatrix} \tag{3.11}$$

The number of weighting coefficients and control points can be very large, but contemporary computers can successfully solve numerically demanding tasks. The estimation can be performed simply by calculating the influence of all the control points weighted by their associated coefficients according to Equation 3.2, as follows:

$$Z=\lambda_1\cdot Z_1+\lambda_2\cdot Z_2+\ldots+\lambda_n\cdot Z_n \tag{3.12}$$

The calculation of the estimation variance includes adding the Lagrange coefficient:

$$\sigma^2=\lambda_1\cdot\gamma(Z_1-Z)+\lambda_2\cdot\gamma(Z_2-Z)+\ldots+\lambda_n\cdot\gamma(Z_n-Z)+m \tag{3.13}$$

Here are shown the two probably most-used kriging techniques. In general, in all linear kriging techniques (since they are constrained optimization problems), the associated equations can be divided into two parts:

a) in one part of the equations, the spatial dependence (spatial correlation) of the measured data is calculated, usually using a variogram;

b) the other part of the equations includes different constraints, resulting in the sum of all weighting coefficient being equal to 1.

4. EXAMPLES OF THE CALCULATION OF KRIGING MATRICES

The model presented in ref.[2] is used as a simple example in the following subsections. There is no reason why this model is better than other similar simple models with several control points, except that the authors have clearly presented all the spatial data values and the variogram values for them. This means that with such a clear and simple model, we can focus in the analysis below on the changes that such data can cause in different kriging technique equations. The calculation tasks are compared using Simple Kriging (best linear estimator, abbreviated BLE) or Ordinary Kriging (best linear unbiased estimator, abbreviated BLUE).

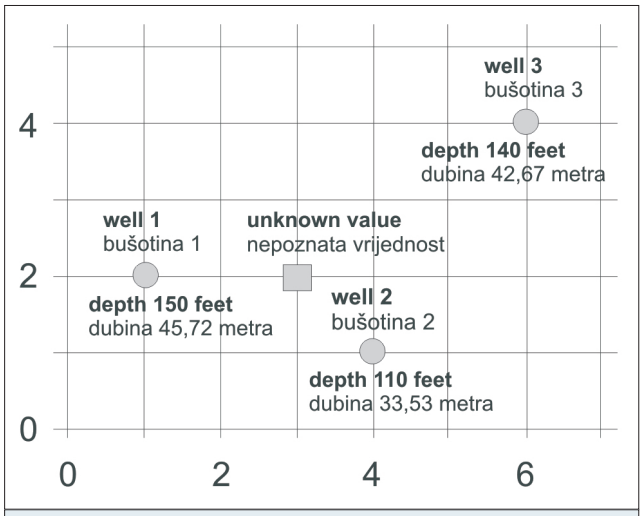

Fig. 1. Distribution of control and estimation points in a coordinate system
Sl. 1. Raspored kontrolnih i točke procjene u koordinatnom sustavu

4.1. Difference in the estimation variance with Simple and Ordinary Kriging techniques

Based on the data for the variogram values for the control points taken from Figure 1 and ref.[2] the matrices for Ordinary Kriging (Equation 3.11) is shown as:

$$\begin{bmatrix}0 & 12.65 & 21.54 & 1\\ 12.65 & 0 & 14.42 & 1\\ 21.54 & 14.45 & 0 & 1\\ 1 & 1 & 1 & 0\end{bmatrix}\cdot\begin{bmatrix}0.3805\\ 0.4964\\ 0.1232\\ -0.9319\end{bmatrix}=\begin{bmatrix}8\\ 5.66\\ 14.42\\ 1\end{bmatrix} \tag{4.1}$$

Matrix [B] can be calculated as:

- In the 1st row:
0x0.3805 + 12.65x0.4964 + 21.54x0.1232 + 1x(– 0.9319)
= 8.001

- In other rows (2nd, 3rd, 4th), the same procedure is applied.

Furthermore, the variance of Ordinary Kriging can be calculated according to:

$$\sigma_{OK}^2=\lambda_1\cdot\gamma(Z_1-Z)+\lambda_2\cdot\gamma(Z_2-Z)+\ldots+\lambda_n\cdot\gamma(Z_n-Z)+m \tag{4.2}$$

This variance is σ^2=6.70 m^2, whereas the standard error is σ=2.59 m. Note that $\sum\lambda=1$ (because of the number of decimal places used, the error is +1‰). Now, Equation 4.1 can be rewritten in the form of the Simple Kriging matrix presented in Equation 4.3 (the locations of the control points are kept the same as in Figure 2):

$$\begin{bmatrix}0 & 12.65 & 21.54\\ 12.65 & 0 & 14.42\\ 21.54 & 14.45 & 0\end{bmatrix}\cdot\begin{bmatrix}0.3805\\ 0.4964\\ 0.1232\end{bmatrix}=\begin{bmatrix}8.939\\ 6.5919\\ 15.3519\end{bmatrix} \tag{4.3}$$

In this matrix, the values of the variograms between the estimation and control points are changed (i.e., values for matrix [B] from Equation 3.3 are changed). This means that the locations of the estimation points could be changed from those in Figure 1. Moreover, it implies that the estimation variance is changed (to $\sigma^2=7.631$ m^2), as well as the standard error ($\sigma=2.76$ m). Both are increased.

4.2. Change in weighting coefficient values in Simple Kriging

Let us now analyse the case in which Simple Kriging maintains the locations of the control and estimation points, as in the previous example. In this way, the same variogram values for all points are held equal in both the kriging techniques examined here. It is clear that the values for the weighting coefficient in Simple Kriging have been changed and can be calculated according the equation:

$$\begin{bmatrix} 0 & 12.65 & 21.54 \\ 12.65 & 0 & 14.42 \\ 21.54 & 14.45 & 0 \end{bmatrix} \cdot \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \end{bmatrix} = \begin{bmatrix} 8.939 \\ 6.5919 \\ 15.3519 \end{bmatrix} \quad (4.4)$$

When this equation is presented as linear formulae, the linear system is:

$$\begin{aligned} 12.65 \cdot \lambda_2 + 21.54 \cdot \lambda_2 &= 8 \\ 12.65 \cdot \lambda_1 + 14.45 \cdot \lambda_3 &= 5.66 \\ 21.54 \cdot \lambda_1 + 14.42 \cdot \lambda_2 &= 14.42 \end{aligned} \quad (4.5)$$

The weighting coefficient can be expressed as:

$$\lambda_2 = \frac{8 - 21.54 \cdot \lambda_3}{12.65} \quad \lambda_1 = \frac{5.66 - 14.45 \cdot \lambda_3}{12.65}$$
$$\lambda_1 = \frac{14.42 - 14.42 \cdot \lambda_2}{21.54} \quad (4.6)$$

The following coefficient values are calculated: $\lambda_1= 0.347$; $\lambda_2 = 0.483$; $\lambda_3 = 0.088$ (note that $\Sigma\lambda= 0.918$). This means that the matrix equation in Simple Kriging for the points distributed as in Figure 1 is:

$$\begin{bmatrix} 0 & 12.65 & 21.54 \\ 12.65 & 0 & 14.42 \\ 21.54 & 14.45 & 0 \end{bmatrix} \cdot \begin{bmatrix} 0.347 \\ 0.483 \\ 0.088 \end{bmatrix} = \begin{bmatrix} 8.939 \\ 6.5919 \\ 15.3519 \end{bmatrix} \quad (4.7)$$

4.3. Calculation of Ordinary Kriging matrices with a regular distribution of control points and variation of the Lagrange multiplicator

In this subsection, we use a new distribution of control points (Figure 2) and new values for the variogram model. The purpose is to present changes in the Lagrange multiplicator and evaluate their influence on the estimated value.

The three examples presented include different multiplicator values. In the first, the Lagrange value is 0.06, taken from published work[3]. However, in the subsequent two examples of kriging calculations, the values for the Lagrange multiplicator are 0.9 and –0.9. These two values are considered the extreme values that the multiplicator can take in practice.

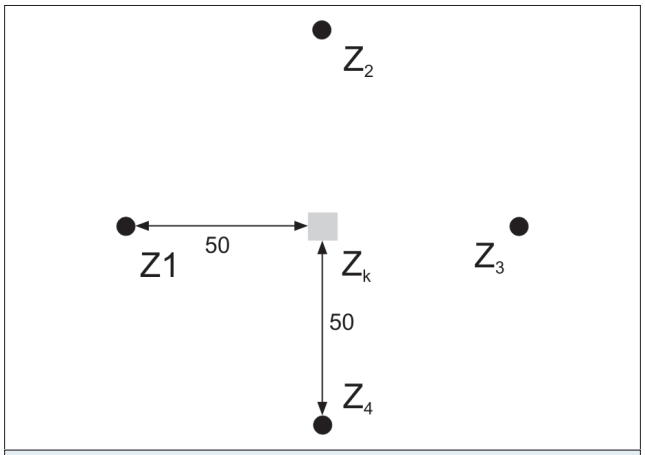

Fig. 2. Regular distribution of the control points
Sl. 2. Pravilan raspored kontrolnih točaka

We selected these three values for the same matrix equations to illustrate the fact that the selection of the multiplicator value is the most important factor in Ordinary Kriging calculations, i.e., in minimizing of the estimation error (kriging variance). The entire calculation is performed manually, which makes it possible to observe the changes in the matrices and linear systems of the kriging (Equations 3.10 and 3.13). The distribution analysed includes four control points. The unknown value is located in the centre of a polygon and the estimation is performed with Ordinary Kriging (Figure 2).

In Figure 2, the relative distances between the control points (50 m) can be read. The variogram values are calculated from these distances. This variogram model has the following characteristics:

- The experimental variogram is approximated by a spherical model;
- The sill is 1;
- The variogram range is 200 m;
- The nugget effect does not apply (0).

4.3.1. Lagrange multiplicator value 0.06

In this subsection, the value of the Lagrange multiplicator is taken from reference[3]. This value allows us to achieve the minimum kriging variance with Ordinary Kriging, which is why we used this value in the manual calculation of the kriging equations and for the calibration calculation performed with different values of the Lagrange multiplicator.

The matrices for Ordinary Kriging in this case are shown as a covariance matrices (inverted to a variogram):

$$\begin{bmatrix} 1.0 & 0.49 & 0.49 & 0.31 & 1.0 \\ 0.49 & 1.0 & 0.31 & 0.49 & 1.0 \\ 0.49 & 0.31 & 1.0 & 0.49 & 1.0 \\ 0.31 & 0.49 & 0.49 & 1.0 & 1.0 \\ 1.0 & 1.0 & 1.0 & 1.0 & 0.0 \end{bmatrix} \cdot \begin{bmatrix} 0.25 \\ 0.25 \\ 0.25 \\ 0.25 \\ 0.06 \end{bmatrix} = \begin{bmatrix} 0.63 \\ 0.63 \\ 0.63 \\ 0.63 \\ 1.0 \end{bmatrix} \quad (4.8)$$

In this example of a regular distribution of the control points, the matrices [λ] and [B] (Equation 3.3) include constant values. If the matrix equation is written in the linear system, it is:

$$\begin{aligned}
&1\cdot 0.25 + 0.49\cdot 0.25 + 0.49\cdot 0.25 + 0.31\cdot 0.25 + 0.06 = 0.6325\\
&0.49\cdot 0.25 + 1\cdot 0.25 + 0.31\cdot 0.25 + 0.49\cdot 0.25 + 0.06 = 0.6325\\
&0.49\cdot 0.25 + 0.31\cdot 0.25 + 1\cdot 0.25 + 0.49\cdot 0.25 + 0.06 = 0.6325\\
&0.31\cdot 0.25 + 0.49\cdot 0.25 + 0.49\cdot 0.25 + 1\cdot 0.25 + 0.06 = 0.6325\\
&1\cdot 0.25 + 1\cdot 0.25 + 1\cdot 0.25 + 1\cdot 0.25 + 0\cdot 0.06 = 1
\end{aligned} \quad (4.9)$$

Now, it is possible to calculate the weighting coefficient and the error variance:

$$\sigma^2_{OK} = 0.25\cdot 0.63 + 0.25\cdot 0.63 + 0.25\cdot 0.63 + 0.25\cdot 0.63 + 0.06 = 0.69 \quad (4.10)$$

4.3.2. Lagrange multiplicator value 0.9

In this example, the Lagrange multiplicator is given a positive vale of 0.9. In such cases, the covariance matrix is:

$$\begin{bmatrix} 1.0 & 0.49 & 0.49 & 0.31 & 1.0\\ 0.49 & 1.0 & 0.31 & 0.49 & 1.0\\ 0.49 & 0.31 & 1.0 & 0.49 & 1.0\\ 0.31 & 0.49 & 0.49 & 1.0 & 1.0\\ 1.0 & 1.0 & 1.0 & 1.0 & 0.0 \end{bmatrix} \cdot \begin{bmatrix} 0.25\\ 0.25\\ 0.25\\ 0.25\\ 0.9 \end{bmatrix} = \begin{bmatrix} 1.47\\ 1.47\\ 1.47\\ 1.47\\ 1.0 \end{bmatrix} \quad (4.11)$$

Again, the matrices [λ] and [B] contain constant values, as in Subsection 4.3.1. These matrices are represented by linear equations in the following system:

$$\begin{aligned}
&1\cdot 0.25 + 0.49\cdot 0.25 + 0.49\cdot 0.25 + 0.31\cdot 0.25 + 0.9 = 1.4725\\
&0.49\cdot 0.25 + 1\cdot 0.25 + 0.31\cdot 0.25 + 0.49\cdot 0.25 + 0.9 = 1.4725\\
&0.49\cdot 0.25 + 0.31\cdot 0.25 + 1\cdot 0.25 + 0.49\cdot 0.25 + 0.9 = 1.4725\\
&0.31\cdot 0.25 + 0.49\cdot 0.25 + 0.49\cdot 0.25 + 1\cdot 0.25 + 0.9 = 1.4725\\
&1\cdot 0.25 + 1\cdot 0.25 + 1\cdot 0.25 + 1\cdot 0.25 + 0\cdot 0.9 = 1
\end{aligned} \quad (4.12)$$

The kriging variance for a Lagrange value of 0.9 is:

$$\sigma^2_{OK} = 0.25\cdot 1.47 + 0.25\cdot 1.47 + 0.25\cdot 1.47 + 0.25\cdot 1.47 + 0.9 = 1.2675 \quad (4.13)$$

4.3.3. Lagrange multiplicator value –0.9

In the last example, the Lagrange multiplicator is given a negative value of –0.9 (our intention was to select a similar value as that applied in Subsection 4.1). Then, the kriging matrices are:

$$\begin{bmatrix} 1.0 & 0.49 & 0.49 & 0.31 & 1.0\\ 0.49 & 1.0 & 0.31 & 0.49 & 1.0\\ 0.49 & 0.31 & 1.0 & 0.49 & 1.0\\ 0.31 & 0.49 & 0.49 & 1.0 & 1.0\\ 1.0 & 1.0 & 1.0 & 1.0 & 0.0 \end{bmatrix} \cdot \begin{bmatrix} 0.25\\ 0.25\\ 0.25\\ 0.25\\ -0.9 \end{bmatrix} = \begin{bmatrix} -0.33\\ -0.33\\ -0.33\\ -0.33\\ 1.0 \end{bmatrix} \quad (4.14)$$

As in the previous two examples, matrices [λ] and [B] have constant covariance values. Moreover, if the matrix is substituted with linear equations, it becomes the system:

$$\begin{aligned}
&1\cdot 0.25 + 0.49\cdot 0.25 + 0.49\cdot 0.25 + 0.31\cdot 0.25 + (-0.9) = -0.3275\\
&0.49\cdot 0.25 + 1\cdot 0.25 + 0.31\cdot 0.25 + 0.49\cdot 0.25 + (-0.9) = -0.3275\\
&0.49\cdot 0.25 + 0.31\cdot 0.25 + 1\cdot 0.25 + 0.49\cdot 0.25 + (-0.9) = -0.3275\\
&0.31\cdot 0.25 + 0.49\cdot 0.25 + 0.49\cdot 0.25 + 1\cdot 0.25 + (-0.9) = -0.3275\\
&1\cdot 0.25 + 1\cdot 0.25 + 1\cdot 0.25 + 1\cdot 0.25 + 0\cdot(-0.9) = 1
\end{aligned} \quad (4.15)$$

The kriging variance is then:

$$\sigma^2_{OK} = 0.25\cdot(-0.3275) + 0.25\cdot(-0.3275) + 0.25\cdot(-0.3275) + 0.25\cdot(-0.3275) + (-0.9) = -0.982 \quad (4.16)$$

All three examples presented in Subsection 4.3 clearly show that the Lagrange value of 0.06 (as given in ref.[3] and shown in Figure 2) is the value at which the estimation variance of Ordinary Kriging is minimal. The reason for this and how we can select the most appropriate value for the Lagrange multiplicator are analysed in the next chapters, the Discussion and Conclusion of the analysis.

5. DISCUSSION OF THE MATHEMATICAL MEANINGS OF THE LAGRANGE MULTIPLICATOR

The results of Chapter 4 clearly show that in the application of ordinary kriging, as a statistical procedure for the estimation of geological or other variables, the value of the Lagrange multiplicator plays a critical role in the final result.

The two accepted values of the Lagrange multiplicator used to minimize the variance in the previous examples differed, with one negative (–0.9319) and the other positive (0.06). The proof that both values are correct is shown by varying of value 0.06 in the kriging matrices (Subsection 4.3). A change in this value induced an increase in the estimation variance (Subsection 4.3.2) or a negative (mathematically impossible) variance (Subsection 4.3.3).

Let us examine once again the mathematical meaning of the Lagrange multiplicator in kriging equations. The value at the estimation point can be expressed as:

$$Z(r) = \mu + \varepsilon(r) \quad (5.1)$$

where

μ is the correct (but really unknown) mean of the entire population;

$\varepsilon(r)$ is the curve and mean value normalized about the value 0 on the curve of the spatial random function.

Usually, we do not know the real mean value of the entire population (μ). Therefore, the estimation is more often performed with the Ordinary Kriging technique than with Simple Kriging, using only the local mean based on data encompassed by the search radius around the estimation point. Moreover, second-order stationarity is also assumed for kriging with the covariance C_Z of the estimation is $Z(x)$. This stationarity can be expressed:

$$C_2(r_1, r_2) = E[\varepsilon(r_1)\cdot\varepsilon(r_2)] = C_2(r_1 - r_2) \quad (5.2)$$

This condition can be described with a variogram (instead of covariance) when the stationarity is presented as:

$$\gamma_Z(r_1, r_2) = \frac{1}{2}\cdot E[\varepsilon(r_1) - \varepsilon(r_2)]^2 = \gamma_Z(r_1 - r_2) \quad (5.3)$$

The array of N measurements $Z(x_1)\ldots Z(x_n)$ at locations $x_1\ldots x_n$ is assumed. Three conditions must be satisfied for an Ordinary Kriging estimation, based on the value of the variable Z ($\hat{Z}$) at any unsampled location x_0:

1. $\hat{Z}$ is linear and calculated from the values $Z(x_1)\ldots Z(x_n)$;
2. $\hat{Z}$ is an unbiased estimation;
3. $\hat{Z}$ minimizes the value of the mean square error expressed as $E\left[Z(x_0)-\hat{Z}(x_0)\right]^2$.

Linearity (condition 1) is realized if the equation $\hat{Z}=\sum_{i=1}^{n}\lambda_i\cdot Z(r_i)$ is satisfied.

Unbiasedness (condition 2) is fulfilled if the following equation is valid:

$$E\left[\hat{Z}(r_0)\right]=\mu\Rightarrow\mu=\sum_{i=1}^{n}\lambda_i\cdot E[Z(r_i)]\Rightarrow\mu=\sum_{i=1}^{n}\lambda_i\cdot\mu\Rightarrow\sum_{i=1}^{n}\lambda_i=1 \quad (5.4)$$

Minimizing the error (condition 3) demands the selection of the most appropriate values for the coefficients $\lambda_1,\ldots,\lambda_n$ and the Lagrange multiplicator $2m$. Their optimization can be expressed for each point as the function $L(\lambda_1,\ldots,\lambda_n,m)$:

$$L=E\left(Z(x_0)-\sum_{i=1}^{n}\lambda_i\cdot Z(x_i)\right)^2-2m\cdot\left(\sum_{i=1}^{n}\lambda_i-1\right)\qquad L\to 0 \quad (5.5)$$

The optimization of the coefficients $(\lambda_1,\ldots,\lambda_n)$ and the Lagrange value (m) is achieved by solving the differential equation $\frac{\partial L}{\partial\lambda_0}=0$.

If we look again at the basic kriging matrices (Equation 3.3) and show them using covariances, the kriging estimation is:

$$C\cdot\lambda_0=C_0 \quad (5.6)$$

The variables C and C_0 can be presented as matrices:

$$C=\begin{pmatrix} C(0) & C(Z_1-Z_2) & \ldots & C(Z_1-Z_n) & 1\\ C(Z_2-Z_1) & C(0) & \ldots & C(Z_2-Z_n) & 1\\ & & \ldots & & \\ C(Z_n-Z_1) & C(Z_n-Z_2) & \ldots & C(0) & 1\\ 1 & 1 & \ldots & 1 & 0 \end{pmatrix} \quad (5.7)$$

$$C_0=\begin{pmatrix} C(Z_0-Z_1)\\ C(Z_0-Z_2)\\ \ldots\\ C(Z_0-Z_n)\\ 1 \end{pmatrix} \quad (5.8)$$

The expected weighting coefficient can then be calculated (using Equation 5.6) as:

$$\hat{\lambda}_0=C^{-1}\cdot C_0 \quad (5.9)$$

The estimation at the selected point is:

$$\hat{Z}(x_0)=\lambda_1\cdot Z(x_1)+\ldots+\lambda_n\cdot Z(x_n) \quad (5.10)$$

The optimal weighting coefficient and Lagrange value allow the calculation of the least possible standard kriging variance using the equation:

$$\sigma(x_0)=C(0)-\lambda'\cdot c_0+m \quad (5.11)$$

6. CONCLUSION

In the previous chapters, we have shown why the Ordinary Kriging technique is more appropriate for the interpolation of point data (compared with Simple Kriging). Moreover, several previous papers have described the application of the kriging method to petroleum geology data (porosity) collected from hydrocarbon reservoirs in the Croatian part of the Pannonian Basin. It was there proven that geostatistical interpolation (as well as stochastic estimation) is the best approach to mapping geological variables (e.g., references [1, 8, 9, 10, 12]).

Based on such analyses, it is concluded that kriging can be usefully applied to cases with a minimum of 10 or even 15 data points. However, any representative statistical dataset of geological variables must include at least 30 data points. This means that we cannot conclude the value of the real population mean (expectation) based only on the usually available datasets. For this reason, the so-called "local mean" is most often applied, which is calculated only from the hard data encompassed by the searching radii, and this favours the Ordinary Kriging technique.

Therefore, we must be very careful to analyse the variables with Ordinary Kriging equations. Most of the variables are the standard elements of all kriging techniques, but there is a unique variable, the Lagrange (linear) multiplicator, the role and importance of which has been discussed in the previous chapters. How can we calculate numerically the most appropriate value for this variable (m), i.e., the value that will result in the least kriging variance?

The answer has been sought in the procedure of random sampling, i.e., the selection of a random seed number from the set of possible (expected) values for the Lagrange multiplicator. It has been shown that this value can be negative, but the values for the kriging variance cannot be negative (mathematically impossible). If the value is randomly sampled many times from some interval (e.g. [–1,1]), one value will produce the least possible kriging variance. It then remains to select the interval width and the number of samplings. How this is done can be described in four steps:

1. Based on experience, it can be assumed that value of the Lagrange multiplicator should occur in the interval [–1,1]. Some values can be very close to 0 (as shown in our example). For these reasons, we consider that the starting point in the random sampling for the Lagrange value should be set at 0.01.
2. In the next step, the starting value must be decreased (in steps of –0.05), i.e., it becomes negative. Again, the appropriate kriging variance can be calculated and registered. Such a procedure should be repeated until the kriging variance is positive. Using this procedure, the value of m with the least kriging variance can be selected (Figure 3 left).
3. The positive side of the Lagrange value should then be checked, again increasing the value in steps of +0.05. Again, a reduction in the variance will be observed, and the procedure should be continued until this reduction vanishes. The first time that the variance increases, the calculation is stopped (Figure 3 right).

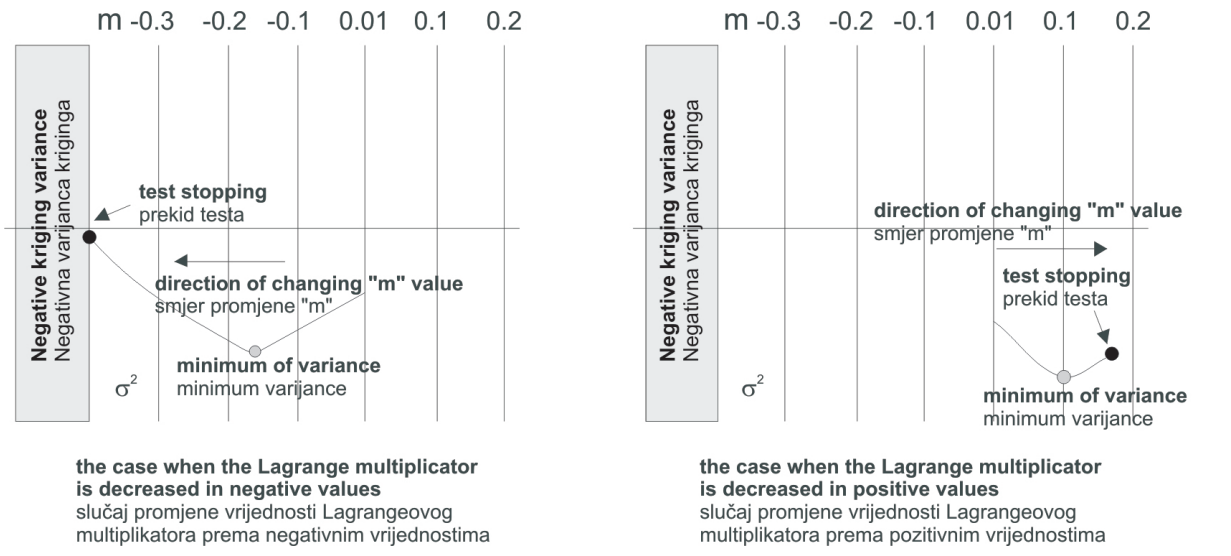

Fig. 3. Graphical representation of how to select the most appropriate value for the Lagrange multiplicator using random sampling
Sl. 3. Slikovni prikaz načina odabira najprimjerenije vrijednosti Lagrangeovog multiplikatora metodom slučajnog uzorkovanja

4. It is important to know that if, for the first positive m (m>0), the variance immediately start to increase, then it can be considered that the minimum kriging variance is found in the negative scale and random sampling can cease (Figure 3 left).

We believe that the four rules discussed above completely describe the correct procedure for selecting the Lagrange multiplicator in Ordinary Kriging equations. Thus, using this technique is one of the best interpolation algorithms for mapping geological variables.

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