Development of a Model Based on the Ordinary Kriging Method for Surface Modeling and Reconstruction from Data Given at Scattered Nodess

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Abstract. This paper studies mathematical equations that can be used to reconstruct and analyze geological surfaces using the data provided at a point (scattered points). The work explains the working capabilities of the kriging technique in the reconstruction of surfaces, what the term signifies as a mathematical model, and how the technique is used in the computing process. The implementation of kriging method in the circumstances of irregularly spaced points of the space is discussed both mathematically and computationally and this example is compared to the case of grid nodes. The findings have revealed that when the points are not distributed consistently, the kriging technique has proven to be a natural and sound mathematical framework in the reconstruction of geological surfaces. This paper is dedicated to the justification of the efficiency of the kriging model in reconstruction and analysis of geological surfaces.

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Key words: scattered nodal points, spatial interpolation, ordinary kriging, semivariogram, surface reconstruction, spatial modeling, interpolation accuracy, mathematical model, function of two variables.

Introduction

The problem of how the values of the unknown intermediate points can be obtained based on known nodal points is of significant scientific and practical importance in interpolation issues and mathematical modeling problems. These issues are common in applied computations, numerical modelling, processing of spatial data, and reconstruction of surfaces of different types [1]. Specifically, the re-construction and analysis of a surface, based on the observation points, is of particular significance in the problems, associated with geological objects. This is due to the fact geological surfaces tend to be complex in nature, their proper definition demands the choice of suitable mathematical models [2]. In this sense, the issue of the construction of a continuous surface out of a set of points is the one among the significant steps in the reconstruction and analysis of the geological surfaces. Interpolation issues are the consideration of structured or grid type nodes in many situations. Spline techniques, and more particularly B-spline techniques, allow the creation of a surface smoothly and accurately in such a situation [3]. The reason is that the nodes are arranged along coordinate directions and it is convenient to build up mathematical models based on tensile products on their basis. This is why in most studies using B-spline methods has become a useful tool in cases where data is provided on a regular or irregular grid nodes with a step-size[4].

Nevertheless, these methods can work well only in situations where the data are pre-geometrically organized. In practice, however, the data are not always provided at grid nodes. Specifically, observation points on geological surfaces can be frequently observed in space in a disordered, haphazard location and can be not based on a pre-determined pattern in particular, when looking at the surface. The distance between the nodes is also different in these situations and the points are not a natural grid of rows and columns. Consequently, it becomes hard to employ classical grid-based methods of interpolation directly. Specifically, when using the

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model of B-splines based on the use of the tensor-product, it is assumed that the data must be in a form of a structure, which does not apply to scattered nodes. Hence, the issue of the reconstruction and analysis of geological surfaces built on the premises of non-continuous spatial points implies a special mathematical solution. In these circumstances mathematical models that consider the spatial dependence between points are particularly important.

One such model is kriging. Kriging is a geostatistical interpolation scheme which derives its primary concept on the premise that values found on points that are close together as far as space is concerned tend to be similar as opposed to those found on distant points [5]. Therefore, when it comes to estimating the value at an unknown point, the observed values are not the only important factor to take into consideration, but also the spatial layout. The biggest merit of the kriging model is that it is properly adapted to the work with the scattered points and the spatial autocorrelation in the estimation of values in the unknown points is taken into consideration [6]. This makes it a difference between it and the simple geometric interpolation methods. Reconstructed surface on the basis of kriging takes into consideration not only values in the known points, but also the statistical relations between them. This is why to data provided at sparse nodes, this method can be considered a natural, well-grounded, and efficient mathematical model of the reconstruction and analysis of geological surfaces. In this paper, mathematical models of the reconstruction and analysis of geological surfaces using data provided at scattered nodes are taken into consideration. Specifically, the practical utilities of the kriging method, the characteristics of the mathematical model, and its efficiency in circumstances of the sparse spatial locations are examined. Moreover, the methodological distinction between the case of scattered nodes and the case of structured grid nodes are also explained and the part played by the kriging model in the reconstruction of geological surfaces is justified.

Inference of data according to the kriging technique.

Let us assume that there are n observation points in the study area, and they are given in the form [6]

$$(x_1, y_1, z_1), (x_2, y_2, z_2), \ldots, (x_n, y_n, z_n)$$

Here, (x_i, y_i) are the coordinates of the observation points, and is the value of the measured parameter at those points. Our aim is to determine the unknown value at the point (x_0, y_0). In the ordinary kriging method, this unknown value can be determined through the weighted sum of known values. The formula of the ordinary kriging method is as follows[6]:

$$\overline{Z}(x_0, y_0) = \sum_{i=1}^{N} \lambda_i Z(x_i, y_i)$$

In this case the λ_i values are kriging weights, and they are calculated through a special system that is founded on spatial dependence. Moreover, in the case of ordinary kriging, $\sum_{i=1}^{N} \lambda_i = 1$ is a condition. This is what makes sure that the estimation is not biased. The Euclidean distances between the points are calculated in the practical implementation of the krige process. The Euclidean formula that is used to calculate the distance between two points is expressed as [7]

$$d_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}$$

whereas the distance between the estimated point and a known point is expressed as

$$d_{i0} = \sqrt{(x_i - x_0)^2 + (y_i - y_0)^2}$$

It requires these distances in the following step to build the semivariogram that represents spatial dependence. In kriging, distance is no longer just a simple geometric value, but it is a way of gauging the extent of statistical similarity or difference between values. The primary aspect of kriging is the semivariogram. It explains spatial autocorrelation of the data i.e. it illustrates the extent to which the values vary with a higher distance. Theoretically, the semivariogram can be described as [8]

$$\gamma(h) = \frac{1}{2} Var(Z(s) - Z(s+h))$$

In practical computation however, the semivariogram of experiment is applied. The calculation is done using the following formula [9]

$$\gamma(h) = \frac{1}{2N(h)} \sum_{(i,j)\in N(h)} (z_i - z_j)^2$$

Here, N(h) the number of pairs of points whose distance is approximately h. That is, each pair of points is placed in groups based on the distance, and the mean of the squared difference of values of each group is computed. By so doing semivariogram points are given. These are the points which are the spatial structure of the data. The points of experimental semivariogram tend to be jagged and hectic. To this end, kriging is no longer performed on the basis of them per se. Rather a theoretical variogram model is fitted on the experimental points. Practically, there is a high level of the application of spherical, exponential, Gaussian, and linear models. Precisely these kinds of semivariogram models are standard options of many software packages used to perform ordinary kriging [10]. The spherical model is written as follows:

$$\gamma(h) = \begin{cases} c_0 + c\left(\frac{3h}{2a} - \frac{1}{2}\left(\frac{h}{a}\right)^3\right), & 0 < h \le a \\ c_0 + c, & h > a \end{cases}$$

The exponential model is as follows:

$$\gamma(h) = c_0 + c\left(1 - e^{-\frac{h}{a}}\right)$$

The Gaussian model is:

$$\gamma(h) = c_0 + c\left(1 - e^{-\left(\frac{h}{a}\right)^2}\right)$$

The linear model is as follows:

$$\gamma(h) = c_0 + bh$$

In this formula, c_0 - is the nugget effect, $c_0 + c$ - is the sill, and a is the range parameter [11]. The nugget is a measure of error in measurement at a very fine scale or of random error at a small scale. The sill shows the higher level in which the semivariogram stabilizes. The range indicates the distance within which the spatial dependence of the points is actually maintained practically. When the distance between the points is larger than the range, then the values are almost independent of one another. One of the most widely applied models in cases of scattered data is the spherical one [12]. Once the semivariogram model of theory is chosen, ordinary kriging weights are determined using a special system of equations:

$$\sum_{j=1}^{n} \lambda_j \gamma(d_{ij}) + \mu = \gamma(d_{i0}), \quad i = 1, 2, \ldots, n$$

$$\sum_{j=1}^{N} \lambda_j = 1$$

μ in this case is the Lagrange multiplier, and this multiplier is added to consider the fact that the weight of the weights should add up to one [13]. After resolving this system weights $\lambda_1, \lambda_2, \ldots, \lambda_n$ are determined. The approximate value at the unknown point is then obtained using them as [14]:

$$\overline{Z}(x_0, y_0) = \sum_{i=1}^{N} \lambda_i Z(x_i, y_i)$$

Analysis and results

Here, the findings of surface reconstruction with the help of ordinary kriging method on the parameters of the data provided at the scattered nodes are presented. The computational experiment used the values developed based on 25 scattered points that were picked on a two-variable test function and an interpolation surface was plotted on them. Consider the following function as a selection function:

$$f(x, y) = \sin(x) \cdot e^{-\cos(y)} + \cos(y) \cdot e^{\sin(x)}$$

Let's select points from this function.

Then, using kriging, we reconstruct the surface in the entire considered domain and compare the results with the real function.

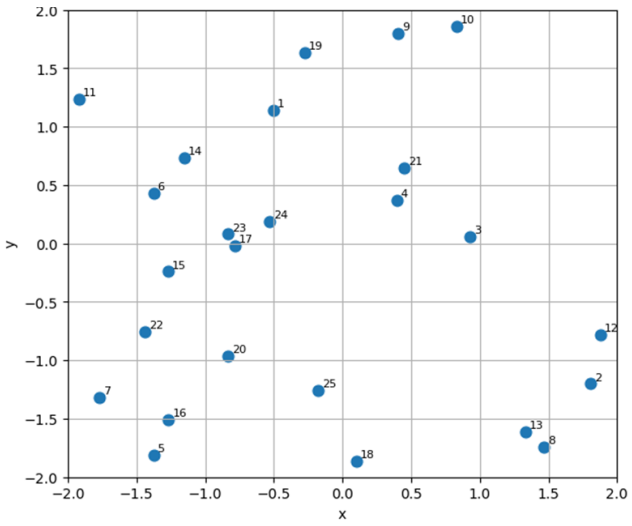

Рис. 1: The location of the selected points in the Oxy plane

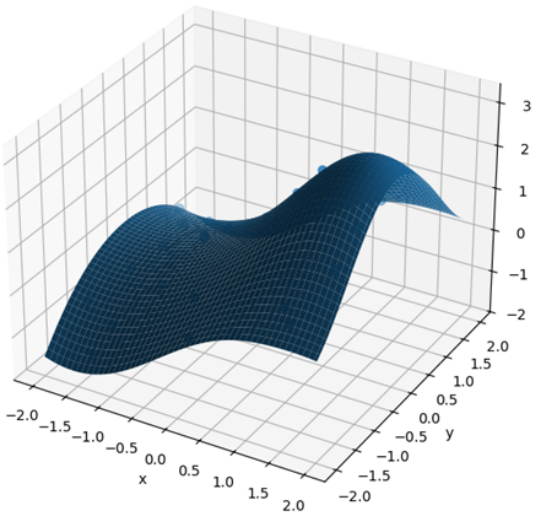

Рис. 2: Graph of the selected function

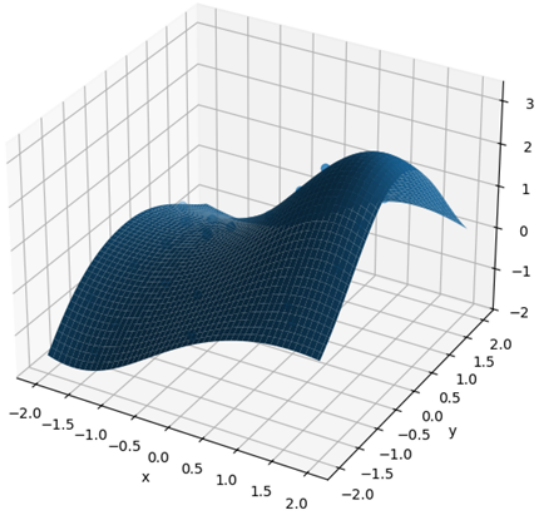

Рис. 3: Surface restored using the Kriging method based on selected points

Таблица 2: Comparison of the original function and Kriging interpolation results

x	y	f(x,y)	Kriging	Error
-2.0000	-2.0000	1.546220	-1.574491	0.028270
-2.0000	-1.1919	0.479171	-0.474588	0.004583
-2.0000	-0.3838	0.013735	-0.012677	0.026413
-2.0000	0.4242	0.011578	-0.050324	0.038532
-2.0000	1.2323	0.518625	-0.534890	0.016273
-2.0000	2.0000	1.546220	-1.128308	0.417912

-1.1919	-2.0000	1.572930	-1.541115	0.031816
-1.1919	-1.3919	0.495756	-0.496400	0.000644
-1.1919	-0.3838	0.011407	-0.002402	0.008995
-1.1919	0.4242	0.013565	-0.012620	0.000945
-1.1919	1.2323	0.535441	-0.516304	0.019137
-1.1919	2.0000	1.572930	-1.280070	0.292861
-0.3838	-2.0000	0.853915	-0.784247	0.069674
-0.3838	-1.1919	0.004355	-0.000882	0.003473
-0.3838	0.3838	0.489445	0.494018	0.004573
-0.3838	0.4242	0.478151	0.475187	0.002964
-0.3838	1.2323	0.040540	-0.037936	0.002407
-0.3838	2.0000	0.835915	-0.854694	0.017876
0.4242	-2.0000	0.004104	-0.043853	0.043850
0.4242	-1.1919	0.842616	0.832229	0.010380
0.4242	-0.3838	1.562313	1.587973	0.025660
0.4242	0.4242	1.540948	1.539491	0.001457
0.4242	1.2323	0.795477	0.832370	0.036893
0.4242	2.0000	0.004104	-0.059993	0.055991
1.2323	-2.0000	0.361279	0.319432	0.041847

Quality of interpolation was measured using the criteria of mean absolute error, root mean square error, root mean square error, maximum absolute error and coefficient of determination.

Comparison and analysis of interpolation performance.

In this experiment, the table of values determined by the test function given was used to restore the surface with the Kriging method based on the table of values. The accuracy of the reconstructed surface was evaluated using several criteria of errors. Specifically, the mean absolute error, root mean square error, root mean square error, the maximum absolute error and the coefficient of determination were determined. By means of these criteria, the closeness of the interpolation results to the actual function was examined. Let us assume that is the true value at the i-th point, and is the value obtained by interpolation. Then the average absolute error is calculated according to the following equation:

$$MAE = \frac{1}{N}\sum_{i=1}^{N}|z_i - \overline{z}_i|$$

This criterion demonstrates the average absolute discrepancy in the true and reconstructed values. The fact that Mae is small means that the total accuracy of the model is good. Based on the results of the calculation, the kriging method MAE amounted to MAE = 0.0219528535. This finding indicates that the values of the reconstruction with the help of kriging were not on average far apart in comparison with the true values of the functions. Thus, the model was accurate enough in the entire domain considered. The low value of MAE

indicates that in data provided at sparsely spaced nodes, ordinary kriging method has the potential to offer consistent and accurate results. The mean squared error is calculated as follows:

$$MSE = \frac{1}{N}\sum_{i=1}^{N}(z_i - \overline{z}_i)^2$$

Since the errors are squared in MSE, larger deviations are evaluated more strongly. For this reason, this indicator reflects well the sensitivity of the model to uneven errors.

The kriging method MSE as per the results of the calculations was MSE =0.0024919208. As usual, in this criterion the squares of the errors are considered and thus the bigger deviations are considered more. The low value of MSE shows that the reconstructed surface of the kriging method is a good fit of the actual surface. Simultaneously, the same result indicates that extremely big errors were not common when interpolating.

Root of the mean squared error i.e. RSME is simply defined as:

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(z_i - \overline{z}_i)^2}$$

The criterion of RSME is quite easy to use in practice, since its unit of measurement is also a unit of the parameter being estimated. This is why RSME can be considered as one of the most significant indicators when the measurement of interpolation accuracy. Based on the results of the calculations, the kriging method RMSE = 0.0499191427. Given that the RSME value will be in the same units as the function being estimated, it is easier to interpret in real life. This finding demonstrates that the values that are obtained by kriging are almost similar to those of the actual values. That is, the mean squared deviation is roughly about 0.05, which is thought to be a small enough error in regards to the test function chosen.

The maximum absolute error is the difference between the result of the interpolation at the worst point and it is denoted as follows:

$$E_{\max} = \max_{1\le i\le N} |z_i - \overline{z}_i|$$

The criterion is particularly significant in the determination of the worst case, as it illustrates the magnitude of an error that can be made by the model at a particular point in the surface.

The results of the calculations revealed that it was equal to

$$E_{\max} = 0.4330520775$$

This indicator is very big compared to the other criteria which implies that there were some local points where significant deviations would have been realized during the interpolation process. That is, in spite of the fact that the overall performance is good, at some stages of the surface the kriging model became less close to the actual function. The main cause of this state of affairs is the sparsity of the nodes structure and lack of the data point density on certain regions. Thus, the supreme absolute error demonstrates that in the commonplace kriging outcome, local errors are not completely eradicated. To determine the overall level of fit of the model, the coefficient of determination i.e. the R^2 indicator was also estimated:

$$\overline{z} = \frac{1}{N}\sum_{i=1}^{N} z_i$$

is the arithmetic mean of the true values. R^2 being near to 1 means that the surface that is reconstructed is very close to the actual function. The results of the calculation were as follows: R^2 = 0.9980582535. The reconstructed surface using ordinary kriging was found to be a good reflector of the overall behavior of the true function since this value is very close to 1. Such a high value of R^2 is a high level of fit of the model. Thus, when the data is provided at separated nodes, ordinary kriging method was used to provide very accurate data in a global perspective.

Conclusion

Taken together, these results show that the ordinary kriging method works well for surface reconstruction based on data given at scattered nodes. In particular, the low values of MAE, MSE, and RMSE indicate that the model has high overall accuracy. The fact that the R^2 coefficient is very close to 1 further shows that the reconstructed surface agrees well with the true function. At the same time, the relatively larger maximum absolute error suggests that some local deviations are still present. Therefore, although ordinary kriging is an effective interpolation method for scattered spatial points, local errors may still occur in certain parts of the surface.

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