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GEOSTATISTICAL ANALYSIS OF VARIABILITY OF SILICA DIOXIDE CONTENT WITHIN LIMESTONE DEPOSIT

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Abstract: In the following paper, the geostatistical analysis of qualitative parameter within a limestone deposit was presented. The parameter was content of silica dioxide. Geostatistical analysis was carried out in order to identify variability of the parameter, what significantly influenced ore exploration. Sampling data was considered with regards to descriptive statistics; logarithmical character of parameter's distribution was indicated. After logarithmical transformation omnidirectional semivariograms were calculated due to the fact that directional anisotropy was not proven. Few theoretical models were fitted to the semivariogram, further on they were verified by means of cross-validation method. Estimation results were obtained by lognormal ordinary kriging technique. They did not confirm that models classified during cross-validation as best fit are also most reliable during estimation. It is recommended to continue research on variability of parameters within the limestone deposit, including analysis conducted by indicator kriging technique. All stages of geostatistical analysis were carried out in Isatis software.

Keywords: geostatistics, variogram modelling, kriging variance, cross-validation, lognormal kriging

1. INTRODUCTION

Conducting mining and geological activities is strictly connected with deposit's exploration, what is being followed by proper identification of parameters variability within the deposit. Very appealing capabilities for description of deposit are given by the geostatistical analysis. This is due to the possibility of a detailed description of changes characteristic. Application of methods for identification of parametrical

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variability makes possible to plan excavations, optimize extraction and also to evaluate resources. The objectives of geostatistical methods applied for mining industry are: analysis of spatial phenomena, correlation between them and using them in order to create three-dimensional models. Geostatistics, as an important tool used by mining engineers, has recently gained on relevance due to being a good indicator of deposit's recognition accuracy. Kriging is a particularly efficient technique. Not only allows on indicating punctual value of variable, but also determines variance, which is the measure of accuracy of performed calculations.

Definition of semivariogram is strictly connected with kriging technique. Semivariogram represents the variability of measured characteristic as a function of variance and distance between observed values (e.g. Journel and Huijbregts, 1978). Semivariogram serves as a source of many relevant data, which are later on used during the stages of fitting the theoretical model. It also makes application of kriging possible.

The objective of following paper is to present the methodology of modelling impurity content in sedimentary rocks. The chemical substance referred to as impurity was silica dioxide. Silica dioxide is not an impurity while producing limestone for the purpose of cement industry. However, silica dioxide is a harmful constituent while producing lime for steel industry or paper fillers (Burnotte and Lauwers, 1998). Another aspect considered within the paper is semivariogram modeling. Particular attention was paid to analysis of criteria for fitting of theoretical models, as well as comparison between theoretical results of estimation and actual results of estimation. The paper is a continuation of research undertaken by the author in the past. The research was conducted for the limestone deposit. The paper is a part of complete variability analysis within this deposit. Numerous authors are undertaking research on geostatistical analysis of qualitative parameters. It is worthwhile to mention authors whose main area of interest is hard coal (Kokesz, 2010; Peroń, 1984; Mucha and Wasilewska, 2005). Spatial variability of sedimentary deposits is analyzed by e.g. (Górska-Zabielska and Stach, 2008).

The research, hitherto carried out on this limestone deposit, indicated a significant variability of manganese oxide, ferrum oxide and sulphur content Variability strongly depended on sample location (stratigraphic unit) (Świtoń, 2014). Furthermore, no correlation between parameters was shown. Due to insufficient number of samples, it was necessary to consolidate stratigraphic units. This consolidation was done by taking into consideration descriptive statistics.

2. GEOSTATISTICAL ANALYSIS – THEORETICAL FOUNDATIONS

In order to use kriging techniques, the definition of semivariogram must be explained. Semivariogram is a graph representing the relation between distance and parametric variance in a certain direction.

The semivariance is calculated by the formula (Deutsch and Journel, 1998):

$$\gamma(h) = \frac{\sum_{n=1}^{N}(z - z')^2}{2n} \tag{1}$$

where:

$\gamma(h)$ - variance of sample pairs located h distance (lag) apart,

z – value at sample z,

z' – value at sample, h distance (lag) apart from z,

n – total number of pairs located h distance (lag) apart.

For each different h distance (lag), a variance γ(h) is calculated. Due to the fact, that drill hole databases often consist of hundreds or even thousands of samples, calculation of semivariance for each distance would require calculating the value according to the Eq. 1. Moreover, calculation of directional semivariograms requires further analysis in order to take the spatial orientation of the vector connecting the pair of samples into consideration.

Creation of variogram requires calculating the semivariance value for around dozen distance lags. For omnidirectional variogram the number of pairs of samples, assuming quite abundant database for the deposit on a relatively small area, will count around several dozen thousands of pairs.

Always a certain tolerance on error is taken into account, because it might be impossible to find a statistically relevant number of samples for absolute values, for example, the constant lag value. In those cases the particular range of values for the allowed search radius of samples pairs is assumed.

The further stage of the geostatistical considerations is to model the variogram in the best possible manner. The variogram might be described by a mathematical model.

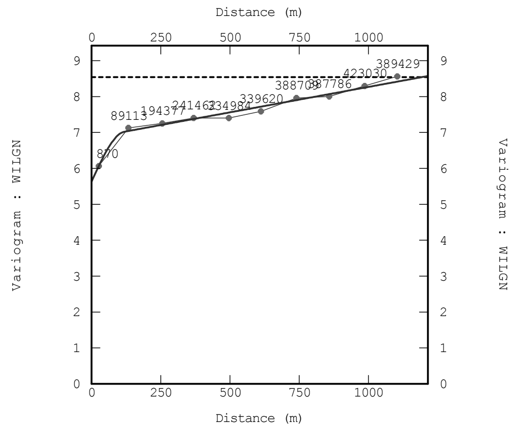


Fig.1. Empirical variogram with fitted theoretical model

In the Fig. 1, the empirical variogram altogether with fitted theoretical model were presented. The parameters of the theoretical model presented in Fig. 1 were generated automatically by the Isatis software. Due to range of variogram's impact, it is possible to choose constrained or unconstrained models. Constrained models are, for example, Matheron's spherical, cubic, stable, exponential and Gaussian, whereas unconstrained are linear, de Wijs or power (Mucha, 1994). It is possible to combine models in order to characterize the flow of the variogram in the best possible way. Variogram's range determines the autocorrelation range, what could be described as a distance up to which theoretical model will have an impact on variability.

2.1. KRIGING EQUATIONS

The next aspect of geostatistical analysis is the proces of estimation of variable value in the centre of block model's cells. The most effective unbiased estimators of a mean value, in the class of linear estimators, are the kriging estimators. The most effective estimator realizes minimum variance of difference between actual parameter's value and its estimated value. In case of ordinary kriging, the most commonly used kriging technique, it is assumed that local means refer strictly to the mean samples. Thus, during assessment of mean value, only the samples in the local neighborhood are taken into consideration (Namysłowska - Wilczyńska, 2006). It means that samples from the given neighborhood are set with proper kriging weights. The kriging weight is how the particular sample influences the final value calculated in the center of block model's cell.

In the ordinary kriging, the value of estimated mean Z^*, in point x_o or in the cell's centre v_o, using data on the basis of n samples located within the given neighborhood, with their linear connection with weights w_a, is being calculated from the formula:

$$Z*(x_0)=\sum_{\alpha=1}^{n} w_\alpha * Z(x_\alpha) \tag{2}$$

In the formula (2) *Z* is the known value of the variable. This formula does not seem overly complicated in computing, but assigning weights to the samples is a difficult task to achieve. The limitation is introduced, that the sum of weights must be equal to 1, because the estimator has to be unbiased. Minimizing the estimation variance with limitation on weights, the system of ordinary kriging is achieved and is represented as a matrix:

$$\begin{bmatrix} \bar{\gamma}(\vec{u}_1,\vec{u}_1) & \bar{\gamma}(\vec{u}_1,\vec{u}_2) & \dots & \bar{\gamma}(\vec{u}_1,\vec{u}_n) & 1 \\ \bar{\gamma}(\vec{u}_2,\vec{u}_1) & \bar{\gamma}(\vec{u}_2,\vec{u}_2) & \dots & \bar{\gamma}(\vec{u}_2,\vec{u}_n) & 1 \\ \dots & \dots & \dots & \dots & \dots \\ \bar{\gamma}(\vec{u}_n,\vec{u}_1) & \bar{\gamma}(\vec{u}_n,\vec{u}_2) & \dots & \bar{\gamma}(\vec{u}_n,\vec{u}_n) & 1 \\ 1 & 1 & \dots & 1 & 0 \end{bmatrix} * \begin{bmatrix} w_1 \\ w_2 \\ \dots \\ w_n \\ \lambda \end{bmatrix} = \begin{bmatrix} \bar{\gamma}(\vec{u}_1,A) \\ \bar{\gamma}(\vec{u}_2,A) \\ \dots \\ \bar{\gamma}(\vec{u}_n,A) \\ 1 \end{bmatrix} \tag{3}$$

Where the left side of the equation represents mean variogram's values for the distances connecting surveying points $\vec{u}_i$ and $\vec{u}_j$, determined on the basis of assumed model of tested parameter's variability. The right side of the equation illustrates differences between each point from the data set $\vec{u}_i$ and the point or area of estimation *A* (Mucha, 1994). In the vector of the variables there are w_n, which are weights given to the samples, and λ is a Lagrange multiplier.

3. APPLICATION OF THEORETICAL KNOWLEDGE TO A CASE STUDY

In the paper, the author aims to present how statistical analysis effects on correctness of results. The other aspect is to show how modeling of empirical semivariograms influences the credibility of kriging results. The analysis was carried out on the limestone deposit, assuming required threshold value of silica dioxide. Maximum allowed content of this chemical substance in the block amounts to 0.85%. This value corresponds to allowed content in the raw material supposed to be used in paper industry.

The discussed limestone deposit is situated in Western Europe. The exact location of deposit will not be mentioned due to confidentiality aspects. Currently, the deposit is not under exploitation; however due to high quality limestone contained within it might be used as a material for production of paper filler. Geologically, the area could be referred to as older carbon rocks. The oldest units were created 350 mln years ago. The deposit is dipping in 63^0 angle, to the north-south direction. It consists of eleven stratigraphic units. One of them is characterized by high content of magnesium oxide, what implies classifying it as dolomite. There is no significant variability of the parameters values within the remaining units. Data about qualitative parameters comes from sixty holes; however, only twelve of them were drilled in order to obtain core data. These holes presented complete geological log. Remaining holes were sampled by destructive drilling, they contained only the averaged data about qualitative parameters. The geological information was missing. After creation of contact zone between unit sit was possible to assign stratigraphy to remaining samples. Average sampling spacing amounted to approximately 70 x 70 m. Sampling was performed in eastern-western direction, in two rows of drillholes dipping in the 40-50^0 angle. Geology of the deposit was regular, units were layered from north to south. After gathering all the data on the stratigraphy, statistical analysis was carried out. The objective of the analysis was to determine the distribution of silica dioxide value.

On the basis of the statistical analysis results it might be concluded that all units are characterized by significant skewness. Logarithmical transformation of variable values
was performed in order to normalize parameter's distribution. In order to achieve this, each value of the variable SiO_2 was calculated as $\ln(SiO_2)$. Descriptive statistics after this transformation are presented in Tab. 1.

Table 1. Descriptive statistics after logarithmical transformation

Unit	Number of samples	Min %	Max %	Mean %	Std. Dev. %	Var. %^{2}	Var. Coeff.	Skewness	Curtosis
A	154	-2.55	1.14	-1.08	0.77	0.60	-0.71	0.57	3.75
B	67	-3.14	1.77	-1.70	0.90	0.82	-0.53	1.72	7.21
C	177	-1.90	2.51	0.18	0.56	0.31	3.13	-0.24	6.88
D	600	-3.91	3.09	-1.68	1.45	2.11	-0.86	0.45	2.38
E	214	-3.51	1.26	-1.06	0.97	0.95	-0.92	-0.46	3.14
F	106	-1.90	1.82	-0.11	0.80	0.64	-7.06	-0.15	3.14
G	100	-1.47	1.96	0.23	0.77	0.60	3.41	-0.06	2.21
H	374	-2.53	2.80	-0.20	0.83	0.68	-4.05	-0.49	3.84
I	133	-2.21	1.98	0.25	0.75	0.57	2.98	-0.02	3.05
J	97	-2.21	1.78	-0.09	1.10	1.22	-11.95	-0.33	1.89
K	152	-3.16	1.67	-1.32	1.27	1.61	-0.96	0.85	2.46

The skewness value diminished significantly after the transformation. In order to simplify further geostatistical modelling, units were consolidated with regards to the skewness. Units with negative skewness value, not lower than -0.5 (units *C, E, F, G, H, I, J*) create one consolidated unit. Unit D, characterized by positive asymmetry and significant number of samples, was considered separately. Remaining units (*A, B* and

K) were characterized by strong asymmetry and therefore were evaluated as an another unit. Even though there is no connection between them it was necessary to analyze them as one domain, due to very little amount of data as well as similar statistical description before transformation. Particular focus later on was paid to modeling of consolidated unit consisting of layers *C, E, F, G, H, I* and *J* in order to model it as precise as it was possible. The consolidated's unit reference number was 2. Its descriptive statistics are presented in Tab. 2.

Table 2. Descriptive statistics for consolidated unit 2

Number	Minimum, %	Maximum	Mean, %	Std. Dev., %
1201	0.03	16.50	1.21	1.23
Variance, $\%^2$	Var Coeff.	Skewness [-]	Curtosis	
1.51	1.02	4.38	37.67	

Logarithmical transformation had another important meaning. It affected on the latter choice of estimation technique.

Frequency histograms of parameter's value before and after the transformation were determined. It may be noticed that before the transformation parameter was highly asymmetric. After transformation its distribution is similar to Gaussian distribution. However, after performing Pearson's compatibility tests, hypothesis on normal distribution was not proven. Histograms are presented in Fig. 2.

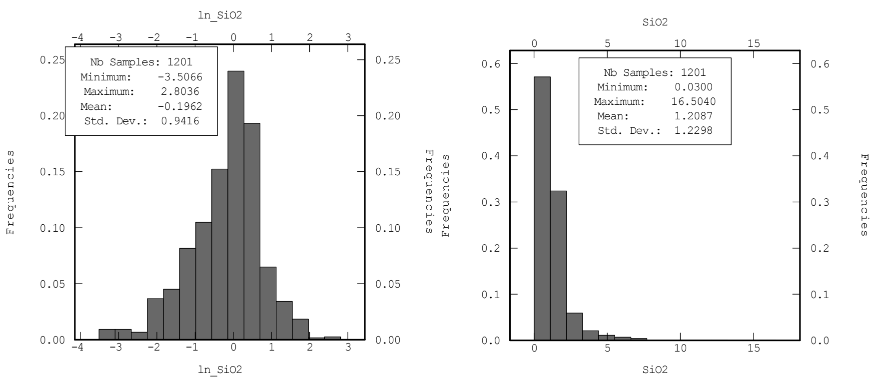


Fig. 2. Frequency histograms of parameter value before and after the transformation

For consolidated unit no directional anisotropy was proven. It was a result of a lack of sufficient amount of data. Omnidirectional empirical semivariogram was calculated instead, as presented in the Figure 3. It is possible to notice an apparent nugget effect. It amounts to 0.25 (standard deviation is equal to 0.5 %). Furthermore, semivariogram is quite regular and it is possible to determine its sill variance. This conclusion serves as a reason to describe a semivariogram by means of mathematical bounded models.

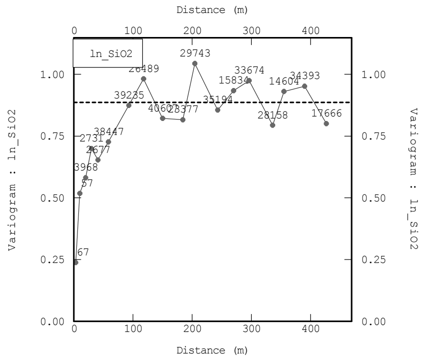
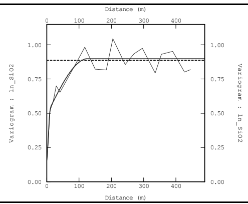
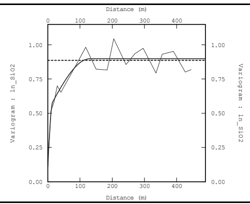
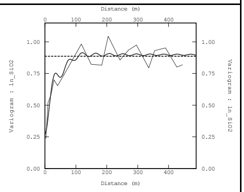


Fig. 3. Omnidirectional empirical semivariogram for SiO_2, unit 2

Nugget effect was also taken into consideration. Compared models consisted of three structures. Obtained parameters of models and fitting critera are highlighted in Tab. 3.

Table 3. Parameters of fitted theoretical models

Reference number of the model	1	2	3
Model type:	Isotropic	Isotropic	Isotropic
Number of structures:	3	3	3
Total number of structure's parameters	5	5	5
Type and parameter value, structure 1:	Nugget effect	Nugget effect	Nugget effect
	Sill=0.15582 $\%^2$	Sill=0.10997 $\%^2$	Sill=0.26944 $\%^2$
Type and parameter value, structure 2:	Cubic	Spherical	Spherical
	Range=15.00 m	Range=130.25 m	Range=125.15 m
	Sill=0.33214 $\%^2$	Sill=0.38259 $\%^2$	Sill=0.33907 $\%^2$
Type and parameter value, structure 3:	Spherical	Spherical	Sine Card
	Range=126.80 m	Range=15.00 m	Scale=142.30 m
	Sill=0.41056 $\%^2$	Sill=0.40540 $\%^2$	Sill=0.28933 $\%^2$
Number of iterations:	35	31	35
Sum of square differences:	0.000178	0.000185	0.000301
Akaike criterium:	-204.384549	-203.651904	-194.388823

Bayes criterium:	-204.277738	-203.545094	-194.282013
Modelled variogram			

All of the models presented in the table are corresponding well with the flow of empirical semivariogram. Particularly important is the range of the model within the distance of 150m, because this distance will be a boundary of the autocorrelation zone. While the theoretical model reaches sill variance value, shape of model at larger distances has no significant impact on the final estimation results. It is important to notice model's fitting criteria in order to compare them at further stages. Model 1 presents the lowest values of Akaike and Bayes criteria as well as sum of square differences, whereas model 3 shows the opposite situation. In this model, all of the mentioned criteria reach the highest value.

In order to verify created models, cross-validation process has been performed. During this process, value of variable is being calculated in the known point, taking into consideration theoretical models. Then, calculated values are compared with assay data. Based on this correlation, it is possible to determine how well theoretical model corresponds with empirical data. One of the indicators informing us whether the model is correct or incorrect is the correlation coefficient. It shows what is the correlation between empirical and estimated values. Different authors state differently (Lawrence, 1989; Rodgers and Nicewander., 1988; Asuero et al., 2006), but it is assumed that correlation coefficient greater than 0.7 represents a situation, when the data is strongly correlated. In case of discussed theoretical models, all of them present a correlation coefficient value greater than 0.7 (Figure 4). Their values are similar. It might be concluded that all of the models are correct and in this case it is impossible to decide which one represents empirical data in the best possible manner.

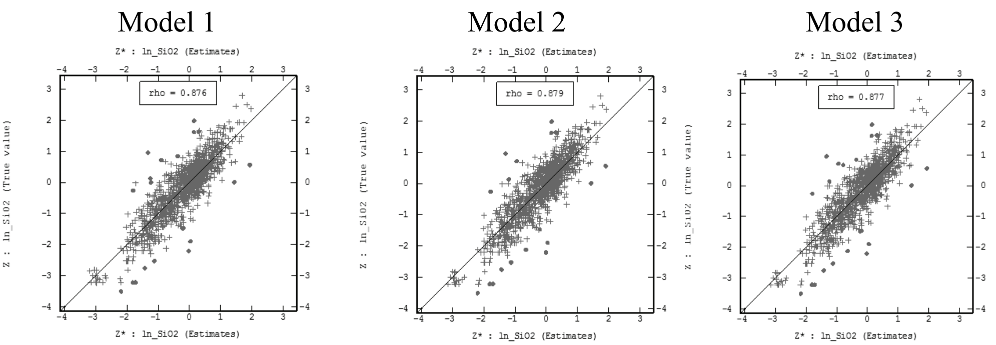


Fig. 4. Scatter plots of true value against estimated value and correlation coefficient

Another aspect considered at this stage of cross-validation was a histogram of relative standard deviation of estimation. It is a foundation for identification of outliers, as well as bias of estimation. Due to the fact that kriging is an unbiased estimator, mean value obtained at the histogram ought to be equal to 0, whereas value of standard deviation should be around 1. Considering these assumptions, it might be evaluated that values of mean and standard deviation are the closest to the above mentioned in model 1. Mean value is close to 0 and standard deviation is 0.9. As it was mentioned before, model 2 seems to be the least reliable, because mean value varies from 0 and standard deviation is the lowest. Histograms of relative standard deviation of estimation are presented in Figure 5.

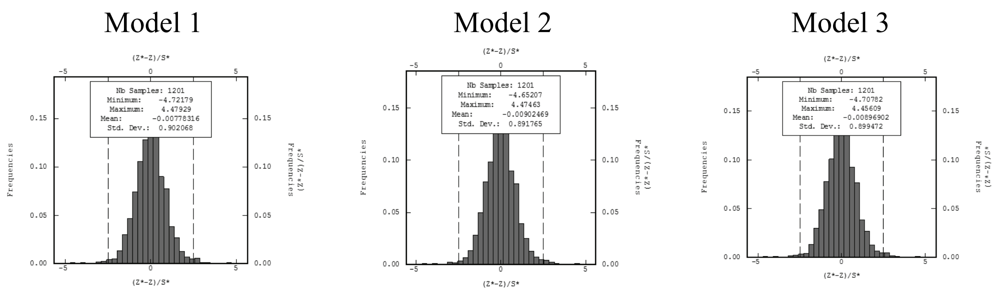


Fig. 5. Histograms of relative standard deviation of estimation

The last aspect considered at this stage of cross-validation was a scatter plot of relative standard deviation of estimation against estimated value. The objective of this scatter plot was to assess the independency of estimated value and estimation error. The aim was to obtain independent values, so their correlation should be close to 0. In case of all models there is no dependency between estimated values and estimation error, as shown in Figure 6. Correlation coefficient value is the closest to 0 is the case of model 1 and, again, model 2 is the least beneficial (even though not significantly).

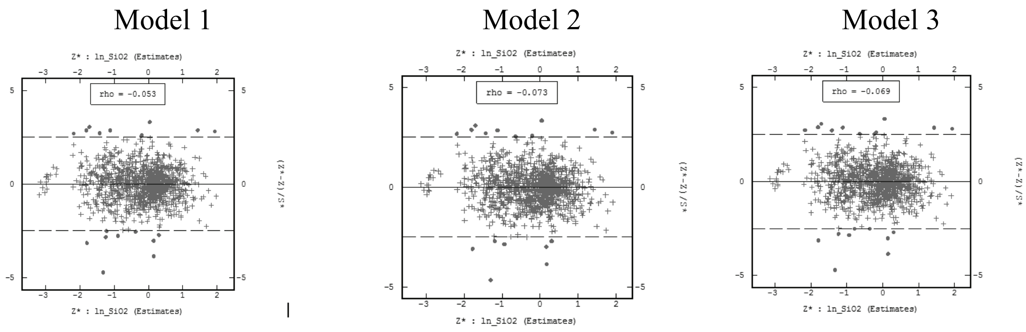


Fig. 6. Scatter plots of relative standard deviation of estimation against estimated value

In order to compare obtained models, estimation within sampling area was conducted. Lognormal block ordinary kriging technique was used due to the transformation carried out previously. Results of estimation are presented in table 4.

Table 4. Estimation results

Variable	Number	Min %	Max %	Mean %	Std. Dev. %	Var. $\%^2$	Var. Coeff.	Skewness	Curtosis
SiO_2* model 1	194132	0.05	10.15	1.19	0.62	0.39	0.52	0.94	4.78
SiO_2* model 2	194132	0.05	8.03	1.21	0.57	0.32	0.47	0.75	3.79
SiO_2* model 3	191432	0.05	7.84	1.21	0.56	0.32	0.47	0.75	3.80
SiO_2 from data	1201	0.03	16.50	1.21	1.23	1.51	1.02	4.38	37.67
Relative std dev. model 1	194132	0.34	1.31	1.06	0.09	0.01	0.08	-1.00	7.08
Relative std dev. model 2	194132	0.40	1.25	1.08	0.07	0.01	0.07	-1.46	9.54
Relative std dev. model 3	194132	0.34	1.20	1.03	0.07	0.00	0.07	-1.91	12.93

After comparing statistics of the model with empirical data it might be noticed that models 2 and 3 represent variable's mean value in the best way. Skewness of the data in all of the models is lower than skewness of empirical data. It proves that kriging has a tendency of "flattening" results. Parameter's spatial variability is represented in the best way in case of model 1; in this model range is the widest and variation coefficient is the closest to the data gathered during sampling.

Standard deviation of kriging was compared as the next aspect. Model 1 presents the highest expected value of standard deviation, which is equivalent with the greatest errors of estimation. Due to this, models 2 and 3 seem to be more appropriate.

It is opposite to the conclusions drawn at the cross-validation stage. It was stated that model 2 was the least satisfying fit. However, the values for all models are similar and it is difficult to state clearly which of the model is the best fit. In conclusion, each of the models could be successfully used in order to run estimation.

4. SUMMARY

Within the paper, the geostatistical analysis of one consolidated unit was conducted. The analysis was concerned on ore dilution by silica dioxide substance. To create the consolidated unit it was necessary to carry out statistical analysis. As its consequence, logarithmical transformation of variable was conducted due to highly asymmetrical distribution of parameter. Logarithmical description of other parameters, within the area of interest, was proven in the previous work dedicated to modeling of limestone deposit. Due to insignificant number of drillholes it was not possible to prove the existence of directional anisotropy. Hence, isotropy of tested parameter was assumed. Variability of parameter was represented by empirical semivariogram. It was described by three complex theoretical models. Range of restricted models equaled to approximately 140m, what determined the autocorrelation zone. Distance between particular drillholes within the structural model was less than 140m. It was concluded that deposit is well explored and further estimation would be reliable. It was also confirmed by cross-validation process, which suggested choosing model 1 as the most reliable. Criteria of fitting theoretical model to empirical semivariogram reached the lowest values in case of model 1. After estimation by lognormal ordinary kriging technique it was confirmed that all of the models provided with reliable results. In case of estimation by lognormal kriging technique bias of estimator might be present. That has an impact on variance of estimation, so in this case it is reasonable to compare relative errors of standard deviation of estimation. It is a better indicator of estimation's quality. Relative errors are the lowest in case of models 2 and 3. However, the differences are slight (up to 0.1%). It is opposite to the conclusions made during cross-validation process. The reason of these discrepancies might be an impact of back-transformation after estimation process. It might be noticed that in case of lognormal kriging, cross-validation might give misleading results. In the following cases discrepancies between results were not significant, but perhaps for semivariograms consisting of more structures the differences might be more apparent.

5. CONCLUSIONS

Based on presented information, it might be concluded that the deposit is well explored. It would be reliable to continue with further estimation of other chemical constituents. Range of silica dioxide content in the model varied from 7.79% (model 3) to 10.10% (model 1). It is significantly lower than the range of this constituent in original data. As a conclusion, conducted estimation eliminated outliers.

Silica dioxide content is important due to further usage of the limestone. In case of paper production, raw material should be characterized by low content of silica dioxide. It might be noticed that in some areas of the described deposit, the material will be unsuitable for production of paper fillers.

In order to perform complete geostatistical analysis, it is planned to run estimations for remaining consolidated units and parameters. Further on, the indicator kriging technique will be applied. It will be applicable to create probabilistic map of the deposit. The other objective of this technique will be a comparison of results.

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