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Coherent Modelling of Mineral Grades and Zones by Coupling Cokriging and Support Vector Machine

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Abstract – The theories of geostatistics and machine learning are originated from statistics, however rooted in different applications. They are sometimes looked as competing theories, sometimes as complementary. The latter perspective is a foundation of this article, which tries to use them jointly to cover their shortages in mineral resources modelling. The theory of geostatistics provides methods for a robust spatial modelling of mineral resources out of univariate and multivariate datasets. However, it demands much effort and experience to generate a coherent model if the dataset contains many categories, either with a single categorical variable or because of crossing two or more categorical variables. This limitation could be covered by machine learning to establish the classification rules between continuous variables and the categorical variables in the space of drillholes. The proposed workflow is applied to a synthetic porphyry copper dataset to verify and illustrate its performance in a multivariate application. The dataset consisting of five mineral grades within five mineral zones. The concluding remark is that the choice of geostatistical interpolator should be done with cautious not to alter the statistical distribution (variance and dimension-support change) of the input core data in the drillhole space while interpolating to the block space.

Keywords**:** lithofacies, geo-metallurgy, classification, mineralization, joint-modelling

1 INTRODUCTION

Backs to 1960s, the theory of geostatistics [1], [2] emerged as a branch of statistics, rooted in the field of mineral resource estimation. It proposes univariate and multivariate interpolation methods to build three-dimensional block model of mineral deposits, conditioned to discrete samples and limited observations. The geostatistical model of a deposit reflects the statistical moments of inputs, i.e. average, variance and histogram, as well as its spatial variability, quantified by variogram function. To model a multivariate dataset, containing correlated or dependent variables, geostatistics proposes some multivariate methods [3] to build a coherent model, e.g. conserving the correlation between the variables and their sum (mineral grades and oxides). Some geostatistical methods are developed to model a continuous variable, like mineral grades: kriging, kriging with external drift, cokriging, Turning Bands Simulation (TBS) and Sequential Gaussian Simulation (SGS) [4].

There are other geostatistical methods for modelling a categorical variable, e.g. facies, mineral zoning, alteration or domaining. Some of the most-used methods are indicator kriging [5], Sequential Indicator Simulation (SIS) [6] and Pluri-Gaussian Simulation (PGS) [7], [8]. If the dataset contains only one categorical variable and several continuous variables, a geostatistical solution might be cascading modelling also named hierarchical modelling, i.e. at first performing modelling of the categorical variable, then replicating the modelling of the continuous variables within each category, e.g. [9]. Cascading results in a coherent modelling between categorical and continuous variables (respecting correlations and proportions). However, in case of having too many categories belonging to one categorical variable or inter-variable categories, e.g. crossing lithology and alteration, the coherent geostatistical modelling demands repeating efforts in variographical and spatial analysis. Thus, combining the geostatistical and machine learning techniques can efficiently join their assets to solve actual mining resource estimation challenges [10].

Whereas geostatistics is powerful in spatial modelling of variables based on the available samples, coordinates, variogram and Euclidean distances; machine learning is powerful in establishing statistical or mathematical relationship between the inputs and the output either continuous (estimation), binary or categorical (pattern recognition). In this article, a supervised pattern recognition is used to link the mineral grades (continuous variables) to the mineral zones (a categorical variable). In addition, machine learning tools and pedagogical documents have been expanded with a high pace, since the end of the twentieth century [11], [12].

This article is a synthesis of some experiences gained on coupling geostatistics and machine learning in modelling mineral resources in which the dataset contains mineral grades (continuous variables) and mineral zones (a categorical variable). The introduced modelling workflow proposes a coherent modelling, i.e. the statistical distributions and correlations observed in the drillhole space are reproduced in the block model. In this regard, multivariate geostatistical techniques are applied to the grade data to generate the block model of grades, then a supervised machine learning algorithm is hired to establish statistical rules between the grades and mineral zones in the input well data, as well as reproducing the mineral zones in the block model. The workflow is implemented in Isatis.neo™ geostatistical software [13], and Scikit learn Python package [14] is used for borrowing the machine learning algorithms for supervised pattern recognition.

2 THEORIES AND WORKFLOW

2.1 Theory of cokriging

Kriging is a geostatistical interpolator for two-dimensional mapping or three-dimensional modelling of a regionalized variable, i.e. a variable defined on a coordinate system. There are several variants of kriging interpolator: simple kriging, ordinary kriging, Eq. (1), block kriging, universal kriging, indicator kriging, etc. The choice of kriging method depends on the variable type (continuous or categorical), its stationarity, c.f. [15], or the change of support [16]. Two main advantages of kriging interpolation compared to the classical interpolators, e.g. inverse distance, is respecting the spatial variability, quantified by variographical analysis, Eq. (2); as well as associating the interpolated value to the expected error of interpolation [4].

$$z_{OK}^{*}(x_0) = \sum_{\alpha=1}^{n} \lambda_\alpha \, z(x_\alpha) \tag{1}$$

$$\gamma(h) = \frac{1}{2N(h)} \sum_{i=1}^{N(h)} [z(x_i + h) - z(x_i)]^2 \tag{2}$$

where the interpolated value at the target position x_0 is specified by the Asterisk, Z_{OK}^{*} (visualized on Fig. 1). The OK represents the method of ordinary kriging. It is the weighted average over n samples, $z(x_\alpha)$, in the vicinity of target of interpolation. The weights, λ_α, are calculated following a matrixial inversion of variographical distances between the positions of samples and the interpolation target. In the method of ordinary kriging, the sum of weights is one that assures an unbiased interpolator. The experimental variogram, $\gamma(h)$, is calculated by $N(h)$ pairs of samples $z(x_i)$ and $z(x_i + h)$, separated by distance h. More details at [17], [18].

Cokriging, Eq. (3), is a generalization of kriging method for modelling a multivariate dataset. It requires a spatial model of coregionalization based on the cross-variogram, Eq. (4).

$$z_{1\,OCK}^{*}(x_0) = \sum_{\alpha=1}^{n_1} \lambda_{1_\alpha} \, z_1(x_\alpha) + \sum_{\alpha=1}^{n_2} \lambda_{2_\alpha} \, z_2(x_\alpha) \tag{3}$$

$$\gamma_{z_1 z_2}(h) = \frac{1}{2N(h)} \sum_{i=1}^{N(h)} [z_1(x_i + h) - z_1(x_i)]\,[z_2(x_i + h) - z_2(x_i)] \tag{4}$$

where z_1 and z_2 are principal and auxiliary variables, respectively. In the method of ordinary cokriging (OCK), the sum of weights of the principal variable, λ_{1_α}, is equal to one; while the sum of weights of the auxiliary variable, λ_{2_α}, is zero to neutralize its impact on the average of the principal variable thus resulting an unbiased interpolation. The experimental cross-variogram, $\gamma_{z_1 z_2}(h)$, is calculated between the regionalized variables. The theory of cokriging could be generalized to more than two variables in the dataset. The advantage of cokriging is reproducing the linear correlations and ratios between the input variables. More details at [3].

2.2 Theory of Support Vector Machine

In the framework of pattern recognition, a classifier establishes some classification rules between input variables (continuous, binary or categorical) and an output categorical variable. A classifier is trained by a supervised learning method, which means the output labels are known in the dataset. There are many methods for building a classifier, e.g. Bayesian (parametric like naïve Bayesian and non-parametric like k-nearest neighbours), decision-tree and Support Vector Machines (SVM) [11], [12].

Each classifier method could be trained on a majority of dataset, while the minority of dataset is reserved for a blind test. The test quantifies the performance of classifier by crossing the observed classes of each test element versus the classification output to produce proportion of correct classification versus misclassification [19]; as well as calculating Classification Correctness Rate (CCR).

In this paper, the SVM classifier is recommended for establishing classification rules between the inputs (mineral grades) and the output (mineral zones). In a simple language, the SVM draws a decision line (in case of two input variables) with the maximum margin from the close observations, called support vectors (Fig. 2). In case of three input variables, a decision surface, and in case of more than three input variables, a decision hypersurface will be defined. The mathematical function of the decision hypersurface could be a linear or a non-linear kernel, e.g. Radial Basis Function (RBF) [20], [21]. Another SVM parameter is a regularization factor (or c), which is a multiplier of loss function versus penalty function that the sum should be minimized [22]. The optimum parameters, including the kernel function and the regularization factor, could be proposed following a series of systematic tests or cross-validation.

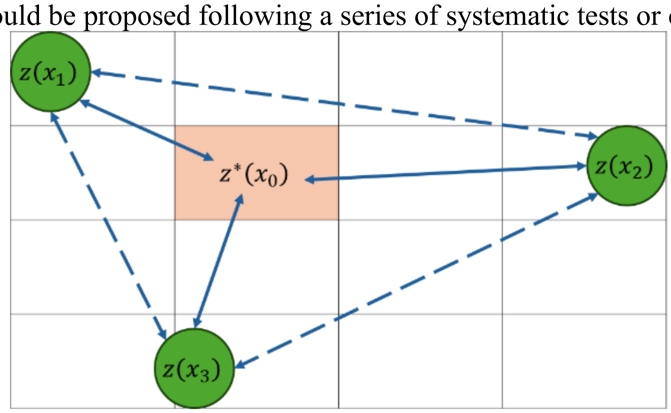


Fig. 1: Interpolation at target position, x_0, based on the samples in the vicinity.

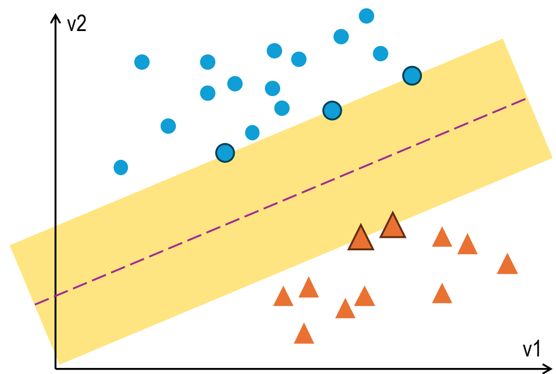


Fig. 2: Schematic representation of SVM classifier, the decision line and the margin oriented by five (2+3) support vectors.

2.3 Workflow of cokriging-SVM

The objective of the cokriging-SVM workflow is to generate a coherent three-dimensional model of mineral resources, conditioned to the mineral grades and mineral zones, known in the drillhole space. The geostatistical methods (cross-variogram and ordinary cokriging) are used to interpolate the continuous variables (mineral grades) in the block space. The SVM classification is used to generate a categorical variable (mineral zones) in block space based on the interpolated mineral grades and the classification rule established in the drillhole space (Fig. 3). The workflow is implemented entirely in Isatis.neo™ which is an independent software for geostatistical methods [13], including cross-variogram and cokriging; and for the SVM classifier, Scikit learn Python package [14], [22], [23] is called through the Python capacity of Isatis.neo™.

3 APPLICATION TO PORPHYRY COPPER MINERALIZATION

3.1 Synthetic dataset

The proposed workflow is applied to a synthetic dataset of porphyry copper, available publicly [24]. The chosen dataset contains 272 wells distanced at about 20 m in densely drilled area, and about 60 m in sparsely drilled area, with total number of 6550 core samples of 10 m length. The selected dataset contains mineral grades (continuous variables) bornite, chalcocite, chalcopyrite, molybdenite and tennantite, as well as mineral zone (categorical variable). The mineral zone contains five Geometallurgical Units (GMU), the statistical distribution of mineral grades in each GMU is visualized in Fig. 4., and their cross-plots are in Fig. 5.

There is a good separation between the GMU5 (non-economic host-rock) and rest of GMUs (Fig. 4). The mineral composition in the oxide and leached zone (GMU1) is different from the sulphide zones (GMU2, GMU3 and GMU4). The three sulphide units have similar mineral composition with some specifications: the supergene zone (GMU2) is rich in chalcocite, the hydrothermal zone (GMU3) is poor in chalcocite and hypogene zone (GMU4) is similar to the hydrothermal zone (GMU3).

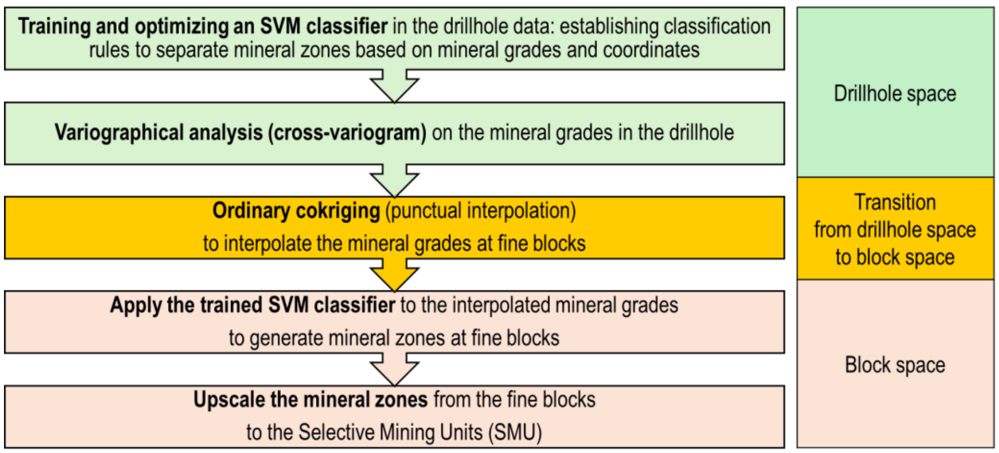


Fig. 3: The workflow of cokriging-SVM.

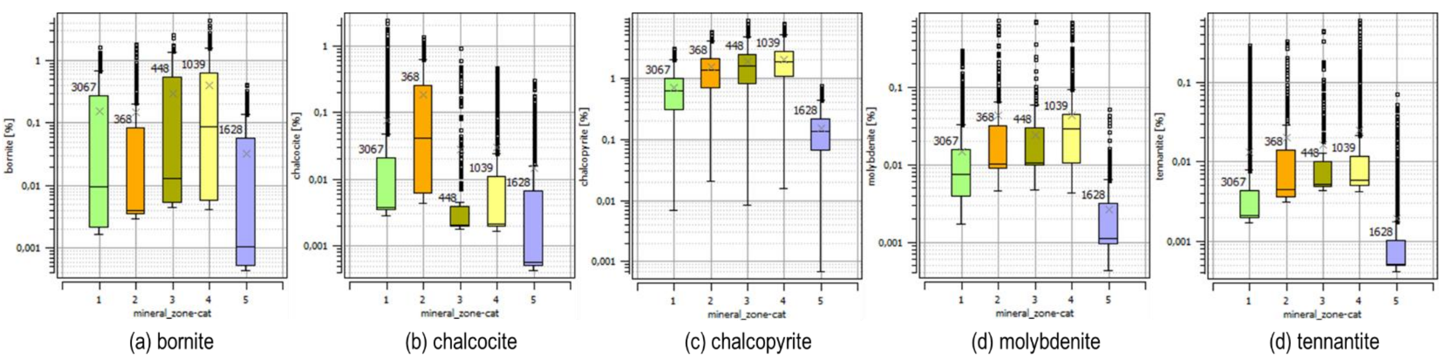


Fig. 4: Statistical distribution of mineral grades in each mineral zone (GMU). The number of samples is mentioned on each boxplot.

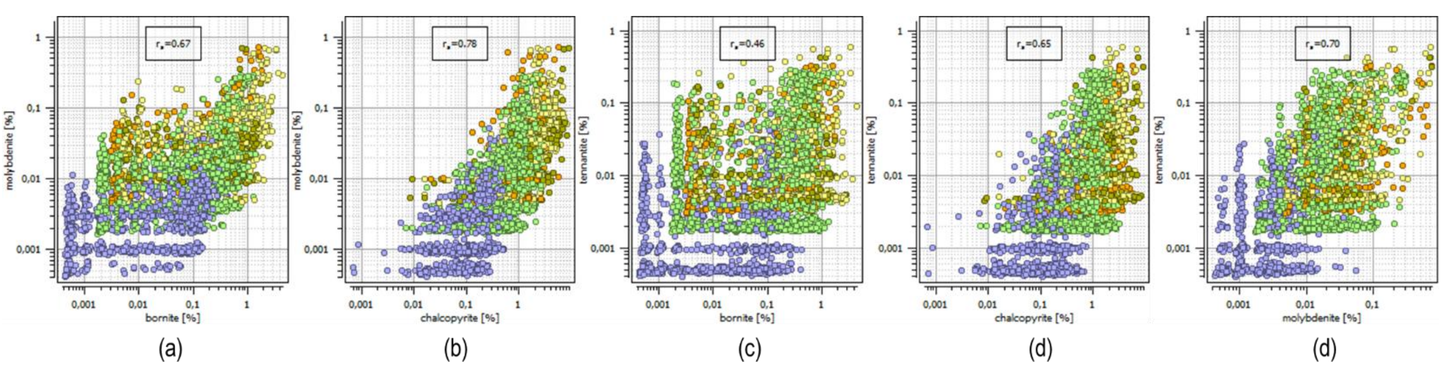


Fig. 5: Correlated mineral grades. The colours correspond to the mineral zones on Fig. 4.

3.2 Training SVM classifier

In the space of drillholes (core samples), the SVM classifier is trained to establish classification rules between eight continuous variables (five mineral grades of Fig. 4, completed by three coordinates x, y and z) as inputs and a categorical variable (mineral zones) as the output. The inclusion of coordinates into the input set is justified by the fact that the mineral zones are geographically distinguishable. The input variables are divided into train and test sets with the proportion of 70% and 30%, respectively. The train-test proportions are kept constant in all the mineral zones. In the train set, each variable is normalized (average to zero and variance to one). In the test set, each variable is normalized according to the average and variance of train set. The normalization guarantees that the difference between the average and variance of input variables does not include biasedness in establishing the classification rules. The parameters of the SVM algorithm should be optimized based on a combination of sensitivity analysis and cross-validation process: In this application, the RBF kernel and the regularization factor of $c = 110$ are found to be the optimal parameters.

The trace elements of the confusion matrix (Table 1) represent the correct classification of each class, ranging from 78% (in GMU3) to 96% (in GMU1), with the average of $CCR = 92\%$. The obtained CCR is much superior to the CCR of the random classification in a five-class problem, i.e. $CCR = \frac{1}{5} = 20\%$. On the confusion matrix (Table 1), the statistics of correct classifications (the elements on the trace) versus misclassifications (the elements out of trace) indicate that the trained classifier is a bit biased toward the GMU1, however this biasedness concerns less than 0.2% of the test set. Worthy to remark that the authors tested the application of some other classification methods too: naïve Bayesian, k-nearest neighbour, decision-tree, logistic regression and the artificial neural network. The choice of the SVM is due to maximizing the CCR.

Table 1: Confusion matrix evaluates the performance of trained SVM on the test set (number of core samples and percentage).

	Classified GMU1	Classified GMU2	Classified GMU3	Classified GMU4	Classified GMU5
GMU1	**883# or 96%**	7# or 1%	4# or 0%	2# or 0%	24# or 3%
GMU2	9# or 8%	**88# or 80%**	0# or 0%	13# or 12%	0# or 0%
GMU3	13# or 10%	0# or 0%	**105# or 78%**	16# or 12%	0# or 0%
GMU4	18# or 6%	11# or 4%	19# or 6%	**264# or 85%**	0# or 0%
GMU5	23# or 5%	0# or 0%	0# or 0%	0# or 0%	**465# or 95%**

3.3 Cokriging

A performant automatic fitting saves time in cross-variogram adjustment between five mineral grades. The fitted model is a nested structure: the nugget effect and two spherical functions with the horizontal ranges of 100 m (short range) and 600 m (long range), and a unique vertical range of 150 m. A selection of cross-variogram plots is provided on Fig. 6.

The cokriging method is applied using punctual mode (no dimension-support change) to prevent variance reduction of mineral grades on the blocks. In this regard, the interpolation target is discretized SMUs. These two considerations are necessary to minimize the variance reduction (smoothness effect) on the block model thus to maximize the generalization ability of the SVM classifier that is trained in the drillhole space. Another consideration is eliminating extrapolation blocks to prevent feeding weak estimation to the SVM classifier. The chalcocite interpolation is plotted on a vertical profile (Fig. 7a), which is consistent with the drillholes patterns. The visualized drillholes are within the lateral extension of 30 m from the profile.

3.4 Applying the trained SVM Classifier to interpolations

The trained SVM classifier with the CCR of 92% is applied to the interpolated values at block space as well as the block coordinates to generate the model of mineral zones. The success of building a coherent model of mineral zone at the blocks depend on the generalization ability of the classifier. Lacking the true mineral zones at the blocks, the visual verification confirms the consistency of the block model of mineral zones with the drillholes (Fig. 7b).

Some local inconsistencies could be observed when comparing the mineral zones in the blocks and in the drillholes: between the elevations 2250 m and 2350 m at the longitude of about 450 m (Fig. 7b). At first glance, a misclassification of GMU4 to GMU2 could be crossed in mind. Further inspection reveals the presence of a drillhole containing GMU2, being masked by another drillhole with GMU4. In addition, 4% of misclassification of GMU4 toward GMU2 is expected according to the confusion matrix of Table 1.

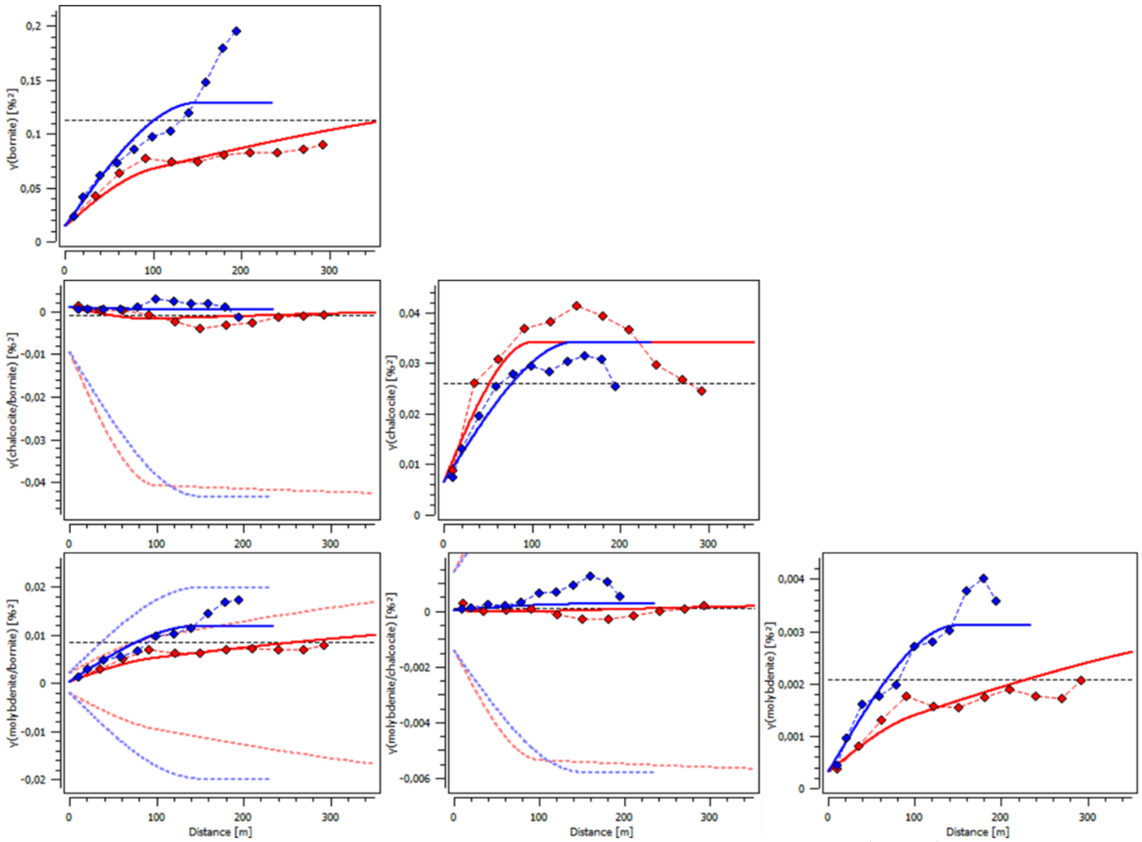
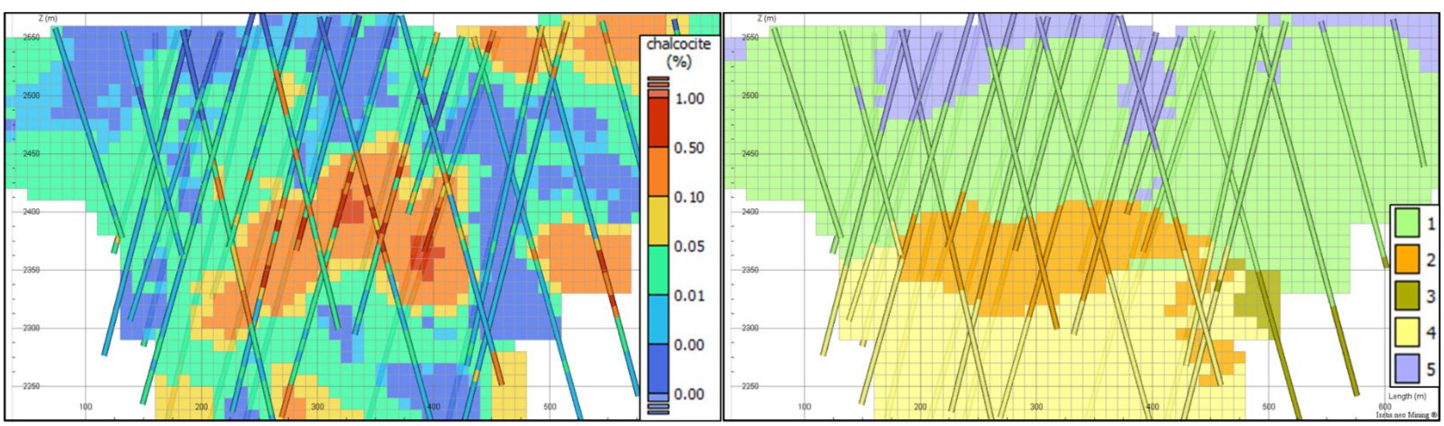


Fig. 6: Selection of cross-variograms: six plots out of total 15 plots: $\binom{5}{1}+\binom{5}{2}=15$.



(a) Cokriging interpolation of chalcocite (b) Mineral zones classified

Fig. 7: Cokriging-SVM outputs on the vertical profile of Y=10 m: cokriging interpolation of chalcocite (a) and mineral zones (b). Lateral extension of drillholes: 30 m.

4 CONCLUSION

The theory of geostatistics has provided powerful tools for multivariate modelling of mineral grades and zones, conditioned to the observations at drillholes. A limitation of geostatistical modelling is in a dataset with too many categories belonging to one variable or when crossing different categorical variables. This limitation could be covered by coupling cokriging algorithm with a classification algorithm (here the SVM is proposed), which results in a coherent block modelling. Worthy to mention that the generalization of a classifier in a new dataset is expected to be less performant than the CCR calculated by the test set, which is statistically very similar to the train set. In this regard, two practical recommendations maximize the generalization ability of the classifier, which is trained in the drillhole space (measured values) and applied to the block space (interpolated values):

- The choice of a coherent multivariate interpolator is important to conserve the mineral grade correlations and ratios in the block space. In this article, cokriging method is used, however there are other alternatives too. The first alternative is using univariate kriging with a unique variogram model for all the mineral grades. The second alternative is using the principal component analysis to decorrelate the inputs. The first alternative is based on a strong variogram hypothesis which alters the spatial correlation of the output. The second alternative ignores the core samples with incomplete grade information. Thus, cokriging remains the best analytical choice if the cross-variogram could be established between the mineral grades.
- The interpolation should not alter the statistical moments of the mineral grades. So, the use of block cokriging (dimension-support change) is not recommended because it reduces the variance of mineral grades in the block space. For the future works, replacing the cokriging with a geostatistical cosimulation which are developed to reproduce the core variance and variogram on the block space even if the drillholes are placed sparsely. In addition, the cosimulation provides the possibility of probabilistic modelling of mineral zones. This concern is a cutting-edge problem for modern mining resource classification problems [25].

The main limitation of the proposed workflow is in a multivariate dataset that the heterogeneity masks the spatial correlation, therefore impossible to perform variogram modelling without separating the categories. The other limitation could be in a condition that the categories result in a non-additive mineral grade, e.g. too much density difference between the categories.

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