# Grade Estimation in Multiple Rock Types Using a Linear Model of Coregionalization for Soft Boundaries

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## Abstract

There are very few instances in nature where hard geological boundaries exist. In most cases, the geological mechanisms that generate a deposit are transitional in nature. Some degree of overlap between geological units can be expected; however, conventional grade estimation usually treats the boundaries between geological units as hard boundaries. This is primarily due to the limitations of current estimation and simulation procedures. The sharing of grade samples across a boundary often has the effect of corrupting the representative statistics of the region of interest, particularly for simulation.

We propose to use a linear model of coregionalization (LMC) to simulate grades using data from adjacent rock types. Although the LMC is traditionally used to characterize the spatial variability of multiple properties in one rock type, we will show that it can be applied to model the spatial variability of one property across the boundary between multiple rock types. Specifically, the cross covariance between two different non-collocated data sets is calculated and the short-scale behavior is extrapolated. This allows inference of the nugget effect of the cross covariance from the nugget effects of the direct covariances. A full model of coregionalization can then be constructed. This model allows the correlation of the grades across the boundaries to be captured through a legitimate spatial model of coregionalization, which can then be used to cokrige or cosimulate grades using data from adjacent rock types. This approach guarantees the correct reproduction of representative statistics of the individual geological units used for resource estimation.

This proposed methodology is applied to a synthetic deposit, and compared to the conventional approach of modeling using hard boundaries. It provides an appealing alternative to capture grade distribution for deposits where complex contacts between different rock types exist. Further, it will improve the resource estimation by reducing the uncertainty in transitional zones around boundaries.

## Introduction

Mineral resource and ore reserve estimation requires a critical decision regarding the geological domains that will be used for the grade modeling, as well as the type of boundaries between these domains. The most common geostatistical techniques, such as kriging and sequential simulation, are based on strong assumptions of stationarity of the estimation domains. The statistical characteristics of one domain can have a very different impact than another domain in the final mineral inventory. Therefore, these domains should be chosen as statistically homogeneous zones, which are geologically significant and coherent, but still holds enough data to allow reliable inference of first and second

order statistics. The domains should also be defined on a scale significantly larger than the selective mining unit (SMU).

Wherever possible, geology should be used to define appropriate estimation domains. Some deposits will have a very simple geometry and mineralisation pattern, making the choice of estimation domains straight forward from geological units. In other cases the mineralisation of interest is not entirely defined by a single geological unit or may transgress their boundaries. In these deposits, it is common to find an important structural or lithological influence on grade distribution and/or multiple events of mineralisation. In these cases, a combination of different geological attributes may reflect an estimation domain. When it is not possible to identify and isolate the geological controls of grade distribution, the estimation domains can defined purely by grade boundaries; however, this method is considerably more dangerous in that under or overestimation of grade and tonnage can result.

Once certain geological or grade boundaries are selected to represent an estimation boundary, the choice should be validated statistically. Differences in the mean, variance and spatial variability between domains are common. A probability plot or a high coefficient of variation may indicate that the chosen domain still has mixed populations. Indicator variograms can be used to test for consistency in anisotropy and grade continuity of different grade ranges within a proposed domain (Guibal, 2001). An analysis on how grades change along a specific domain boundary is quite useful to validate a proposed boundary and determine the nature of the domain boundary. Also used to validate the choice of geological domains are several data analysis techniques, including cluster analysis, principal component analysis, discriminant analysis, characteristic (Botbol, 1971) analysis. Care must be taken when using these techniques since none of these considers spatial correlation component, which is critical in a geostatistical study.

#### Modelling grades given a boundary

Domain boundaries are often referred to as either 'hard' or 'soft'. Hard boundaries do not permit the interpolation or extrapolation of grades across domains. Soft domain boundaries allow grades from either side of a boundary to be used in the estimation of each domain.

For deposits with hard domain boundaries, such as coal seams or sedimentary zinc deposits, the definition of domain boundaries is relatively straightforward. For deposits with soft domain boundaries, such as some porphyry Cu-Au deposits where the disseminated mineralisation has a gradational nature, boundaries separating ore from waste and from one zone to another may be diffused or transitional.

Once the estimation domains are established, either deterministically or stochastically, if the boundaries of the domain are considered to be 'hard', the estimation of the domain is straightforward, using only the samples within the domain, since no interpolation across domains is allowed. If any of the boundaries of a domain are considered to be 'soft', then the common practice is to share samples (from the conditioning data and/or from previously simulated nodes) within a given extent of influence of one domain over the other. The 'outside' samples are treated equal to those within the domain, that is, the same mean, variance and covariance model from the samples within the domain are assumed. This generally has the effect of corrupting the representative statistics of the domain of interest. This corruption of the final grades, especially in the transition zones, often dissuades practitioners from handling these boundaries as soft boundaries and the result is that the boundaries are left as 'hard' boundaries. Nevertheless, the nature of the geological processes of mineralisation generates some degree of overlapping between units, and 'soft' boundaries are probably far more common than 'hard' boundaries. Even so, when the domains are defined purely by grade, it is highly recommended to use at least a one-way soft boundary to account for possible dilution; data within the high-grade domain is not used to estimate an adjacent low-grade domain, but for the estimation of the high-grade domain, data from the low-grade domain is used (Glacken and Snowden, 2001).

We propose to use a linear model of coregionalization (LMC) to simulate grades using data from adjacent domains. Although the LMC is traditionally used to characterize the spatial variability of multiple properties or metal grades in *one* domain, we will show that it can be applied to model the spatial variability of *one* property across the boundary between *multiple* domains. A full model of coregionalization allows us to capture the spatial correlation of grades across the boundaries through a legitimate spatial model, that can later be used to cokrige or cosimulate grades using data from adjacent domains. This approach guarantees the correct reproduction of representative statistics of each geological domain.

#### Theoretical Background

Consider that the outcomes of our variable of interest (e.g. metal grade) in any of *K* geological domains correspond to the random variable  $Z_k$ , with k=1,...,K, and each of them is second order stationary within its domain.  $Z_k$  can be considered as linear combinations of *n* independent random variables  $Y_i$  which follows normal distributions with mean  $m_i$  and standard deviation  $\sigma_i$ , with i=1,...n.

$$\mathbf{Z}_{\mathbf{k}} = \sum_{i=1}^{n} a_i \mathbf{Y}_i \quad \forall k$$

The mean and variance of  $Z_k$  are:

$$E\{\mathbf{Z}_{k}\} = m_{k} = \sum_{i=1}^{n} a_{i}m_{i} \quad \forall k$$
$$E\{(\mathbf{Z}_{k} - m_{k})^{2}\} = \sigma_{\mathbf{Z}_{k}}^{2} = \sum_{i=1}^{n} a_{i}^{2}\sigma_{\mathbf{Y}_{i}}^{2} \quad \forall k$$

The covariance of  $Z_k$  at a vectorial distance **h**, can also be calculated as an expression of the coefficients  $a_i$  and the covariances of  $Y_i$  for i=1,...n:

$$Cov_{\mathbf{Z}_{k}}(\mathbf{h}) = \sum_{i=1}^{n} a_{i}^{2} Cov_{\mathbf{Y}_{i}}(\mathbf{h}) \quad \forall k$$

Similarly, the cross-covariance of  $Z_k$  and  $Z_m$ ,  $\forall k \neq m$ , with k,m=1,...,K can also be derived as an expression of the coefficients  $a_i$  for  $Z_k$ , and  $b_j$  for  $Z_m$ , i,j=1,...n,

$$Cov_{\mathbf{Z}_{k}\mathbf{Z}_{m}}(\mathbf{h}) = E\left\{\sum_{i=1}^{n} a_{i}\mathbf{Y}_{i}(\mathbf{u})\sum_{j=1}^{n} b_{j}\mathbf{Y}_{j}(\mathbf{u}+\mathbf{h})\right\} - E\left\{\sum_{i=1}^{n} a_{i}\mathbf{Y}_{i}(\mathbf{u})\right\} \cdot E\left\{\sum_{j=1}^{n} b_{j}\mathbf{Y}_{j}(\mathbf{u}+\mathbf{h})\right\}$$
$$= \left(\sum_{i=1}^{n} a_{i}b_{i}E\left\{\mathbf{Y}_{i}(\mathbf{u})\cdot\mathbf{Y}_{i}(\mathbf{u}+\mathbf{h})\right\} + \sum_{i=1}^{n}\sum_{j\neq i}^{n} a_{i}b_{j}E\left\{\mathbf{Y}_{i}(\mathbf{u})\cdot\mathbf{Y}_{j}(\mathbf{u}+\mathbf{h})\right\}\right)$$
$$-\left(\sum_{i=1}^{n} a_{i}b_{i}E\left\{\mathbf{Y}_{i}(\mathbf{u})\right\} \cdot E\left\{\mathbf{Y}_{i}(\mathbf{u}+\mathbf{h})\right\} + \sum_{i=1}^{n}\sum_{j\neq i}^{n} a_{i}b_{j}E\left\{\mathbf{Y}_{i}(\mathbf{u})\right\} \cdot E\left\{\mathbf{Y}_{j}(\mathbf{u}+\mathbf{h})\right\}\right)$$

But since  $\mathbf{Y}_i$  is independent of  $\mathbf{Y}_j$  there is no cross spatial correlation between  $\mathbf{Y}_i(u)$  and  $\mathbf{Y}_j(u+h)$ , i.e.,  $E\{\mathbf{Y}_i(u) \cdot \mathbf{Y}_i(u+h)\} = E\{\mathbf{Y}_i(u)\} \cdot E\{\mathbf{Y}_i(u+h)\}$ ,  $\forall i \neq j$ .

$$Cov_{\mathbf{Z}_{k}\mathbf{Z}_{m}}(\mathbf{h}) = \sum_{i=1}^{n} a_{i}b_{i}E\left\{\mathbf{Y}_{i}(\mathbf{u})\cdot\mathbf{Y}_{i}(\mathbf{u}+\mathbf{h})\right\} - \sum_{i=1}^{n} a_{i}b_{i}E\left\{\mathbf{Y}_{i}(\mathbf{u})\right\}\cdot E\left\{\mathbf{Y}_{i}(\mathbf{u}+\mathbf{h})\right\}$$
$$= \sum_{i=1}^{n} a_{i}b_{i}Cov_{\mathbf{Y}_{i}}(\mathbf{h})$$

To illustrate the concept above, lets consider a 2D example with only two domains,  $Z_1$  and  $Z_2$ , constructed using the following underlying non-standard normal random variables:

$$Y_{1} \sim N(0.5, 0.5) \text{ with } Cov(h) = 0.05 + 0.45 \cdot Sph_{\substack{hmax=200\\hmin=200}}(h)$$
$$Y_{2} \sim N(2.0, 1.0) \text{ with } Cov(h) = 0.1 + 0.9 \cdot Sph_{\substack{hmax=50\\hmin=300}}(h)$$
$$Y_{3} \sim N(1.0, 0.5) \text{ with } Cov(h) = 0.05 + 0.45 \cdot Exp_{\substack{hmax=400\\hmin=100}}(h)$$

With the following coefficients *a<sub>i</sub>* and *b<sub>i</sub>*:

$$a_1 = \sqrt{0.5}$$
  $b_1 = \sqrt{0.5}$   
 $a_2 = \sqrt{0.5}$   $b_2 = 0.0$   
 $a_3 = 0.0$   $b_3 = \sqrt{0.5}$ 

The theoretically derived cross-covariance between  $Z_1$  and  $Z_2$  was checked against 10 different realizations obtained from unconditional simulations of  $Y_1$ ,  $Y_2$  and  $Y_3$ . Three different spatial arrangement for  $Z_1$  and  $Z_2$  were considered: (1) collocated (just as a check), (2) the two domains adjacent to each other (Fig. 1A), and (3) the two domains merged (Fig. 1B) using a categorical binary model obtained via a Boolean simulation program, ellipsim, that generate a 2D map of ellipsoids of variable size and anisotropies for a given target proportion (Deutsch and Journel, 1998).



Fig. 1: Example of two domains: (A) the domains are side by side,  $Z_1$  correspond to the right-half and  $Z_2$  to the left-half, (B) the two domains are merged using a categorical binary model.  $Z_1$  shows anisotropy along the X-axis, which have on average lower values than  $Z_2$ , which shows anisotropy along the Y-axis.

The cross-covariance between  $Z_1$  and  $Z_2$  when both variables are collocated match almost exactly, as shown in figure 2 the average variogram over all realizations is very close to the analytical model. This is expected given that the analytical model was derived from the covariance models of  $Y_1$ ,  $Y_2$  and  $Y_3$ , and the corresponding coefficients. The ergodic fluctuations associated with the different realization show a very low dispersion.



Fig. 2: Cross-covariance reproduction of the simulated random variables  $Z_1$  and  $Z_2$ , assuming both variables are collocated. The dots are the average taken over all realizations; individual realizations in dashed lines; and the thin red solid line correspond to the analytical model. The analytical model is very close to the average over all realization, which can make difficult to differentiate the dots from the solid line.

In the case where the two domains are side by side, the simulated values corresponding to the average overall realizations, follow the analytical model fairly well (Fig. 3A), although configurations where the boundary is parallel to the major anisotropy of one of the domains ( $Z_2$  in this case), showed a systematically lower covariance at shorter lag

distances than the theoretical model, and greater ergodic fluctuations at lag distances near zero. This latter observation means that inference of the nugget effect of the cross covariance is more uncertain in geometrical configurations similar to this one.

For the second scheme, using a circular shape with radius of 150 meters and three target proportions of  $Z_1$  (25, 50 and 75%), the cross covariance between the experimental points derived from the average over all realizations compares well with the analytical model (Fig. 3B). Contrary to the side-by-side scheme, the fluctuations at short lag distances have a smaller range of variation, and a wider range of variation at distances beyond the range of correlation. Therefore we can expect that when more contact surfaces between domains are available and are more irregularly oriented, the determination of the nugget effect should have less uncertainty, compared to the case where a single contact surface existed between two domains, especially if it is oriented parallel to the direction of major anisotropy of the values of one of the domains. A completely straight or planar boundary gives the least possible surface area to the boundary. This leads to the smallest possible transition zone between rock types and the fewest possible pairs for variogram calculation. This was also confirmed by a poorer reproduction at shorter lag distances, with lower covariances than the analytical model, when the target proportion of the domain  $Z_1$  was lower than 10%.



Fig. 3: (A) Cross-covariance between  $Z_1$  and  $Z_2$  combined side by side. (B) Cross-covariance between  $Z_1$  and  $Z_2$  combined using ellipsim categorical model as a boundary model with a target proportion of  $Z_1$  of 50%. The dots are the average taken over all realizations; individual realizations in dashed lines; and the thin solid line correspond to the analytical model.

Using the same synthetic examples, the impact of different drill hole data spacing was examined. Overall the reproduction of the cross covariance analytical model is fairly good, although a wider range of fluctuation between realizations is observed. If the grid or data spacing is larger than the range of the cross-covariance between data from the two domains, the calculation of a cross-covariance will be meaningless. Also the grid spacing will be critical if there are insufficient pairs to infer a model.

#### Application

A synthetic example was created in order to use a full LMC cosimulation and compare it with the results obtained from simulating two adjacent rock types independently. The LMC model was obtained by calculating the cross variograms between values of the different domains and the direct variograms within each rock type.

Using a similar scheme as the previous example, the linear combination of three underlying random variables were used to populate a synthetic geological model; this will be consider as the 'true' image for comparison. The 2D reference image (2000 by 1000 meters, with a 10 meters grid spacing in both directions) was sampled at a spacing of 70 meters in the X-direction yielding a total of 2800 samples.

Variograms were calculated from the normal scores transform values from each rock type, **RT1** and **RT2**. Cross variograms can not be calculated if the variables are not collocated, which is the case here since we are trying to characterize the spatial variability across the boundary between **RT1** and **RT2**. An alternative (Wawruch *et. al.* 2003) is to calculate the cross covariance between the variables by (1) extrapolating the experimental points at lags near to zero to obtain the structured cross covariance ( $B_{Z1-Z2}$ ) (Fig. 4), (2) determining the relative nugget effects **Z**<sub>1</sub> and **Z**<sub>2</sub>, and (3) calculating the sill of the cross variogram between **Z**<sub>1</sub> and **Z**<sub>2</sub> as:

$$Cov_{z_{1}-z_{2}}(0) = \frac{B_{z_{1}-z_{2}}}{1 - \left[\frac{1}{2}\left(\frac{Cov_{z_{1}}^{0}}{\sigma_{z_{1}}^{2}} + \frac{Cov_{z_{2}}^{0}}{\sigma_{z_{2}}^{2}}\right)\right]}$$

In this example, the relative nugget effects obtained from the direct variograms of each rock type were both 0.1, the structured cross covariance was chosen at 0.4, so the sill of the cross variogram is 0.44. With this value the experimental points from the cross covariance can be inverted to obtain the cross variogram between  $Z_1$  and  $Z_2$ . Although the nugget effect between the grade at each side of the boundary is not needed in any calculations because there is no collocated data nor we estimate collocated grid blocks; most cokriging and cosimulation programs require the LMC to be defined with variogram models, which requires the nugget effect and the sill of the cross variogram.



Fig. 4: Sketch with the structured cross covariance and calculated sill of a cross variogram given an experimental cross covariance between two non-collocated variables.

The direct and cross variograms of  $Z_1$  and  $Z_2$  were model using a linear model of coregionalization (LMC) obtained by a semi-automatic variogram fitting program (Larrondo *et. al.*, 2003). Since independent simulations of  $Z_1$  and  $Z_2$  were also performed, the direct variograms of each variable were modeled independently.

The cosimulation was performed using the full LMC cokriging option of the ultimate sgsim program (Deutsch and Zanon, 2002); in this case each rock type was simulated using the samples of the other rock type, as a secondary variable. For the comparative case, sequential gaussian simulation was used to simulate each rock type independently as the contact between **RT1** and **RT2** was a 'hard' boundary.

The reproduction of the direct variograms, both for the cosimulation or independent simulation schemes, was fairly good. Although the reproduction of the cross variogram was poor compared with the analytical model, the first 100 meters (total range) in the X-direction showed a similar amount of correlation (Fig. 5). The case where the contact between **RT1** and **RT2** was assumed to be a 'hard' boundary, resulted in almost no correlation for lags less than the range of the cross variogram, even though the reference map was correlated between boundaries by construction. While for a 'soft' boundary assumption, the correlation for shorter lag distances of the average over all realization is closer to the correlation shown by the 'truth' reference.



Fig. 5: Cross covariance reproduction for  $Z_1$  and  $Z_2$ , cosimulated (right) and independently simulated (left). In a 'soft' boundary scheme (right) the correlation between the simulated values is very close to the 'truth' reference. In the contrary, in a 'hard" boundary assumption, the correlation at short lag distances is significantly lower. The dots represent the average of simulated values over ten realizations, the dash line correspond to the cross covariance calculated for the training image, and the solid line is the analytical model derived from the theoretical expression.

Cross validation of the model obtained by independently simulating  $Z_1$  and  $Z_2$  showed that, given the parameters used, the model is accurate and precise (Deutsch 2002). The cosimulated model is also accurate, and equally precise for **RT1**, while for **RT2** is slightly less precise than the model obtained from independent simulations. This is not surprising since the fitted LMC model for this rock type did not fit the data as well as for **RT1**, but this is a common disadvantage when using a linear model of coregionalization instead of independent spatial model. The cosimulated model did, however, show less smoothing (Fig. 6) and a lower standard deviation of the error (true-estimated) than the independent

simulation scheme (0.5 versus 0.85 on average between the two rock types). This translates to less conditional bias in the estimation.



Fig. 6: Cross validation of data values in **RT1** and **RT2**, estimate independently (left) versus cosimulated (right). The cokriging cross validation show far less conditional bias than the estimation of each rock type independently, especially for **RT2**.

The cumulative distribution of back transformed simulated values to original units, showed a very good reproduction of the data, under both schemes. The target mean and variance are well reproduced for both cosimulation and independent simulations, even though the variance shows a greater mismatch with the conditioning data in the case where cosimulation was used.

## Comparison at the boundary

In order to compare the performance of the two methods, we need to focus on the results near the boundary where we can expect to have greater differences.

One comparison was done using the expected value (E-type value, Deutsch and Journel, 1998) in original units at each location and compare it with the 'true' value in the reference map. The expected value is obtained by averaging the simulated value of all realizations at each location. Comparing blocks within a given distance from the boundary, both

simulation schemes give similar results, but the block values obtained from cosimulation show higher correlation coefficients with the true values. As expected, the difference between the two methods becomes smaller beyond the range of correlation of the cross variogram (Fig. 7).



Fig. 7: Correlation coefficient between E-type estimates of cosimulated and independently simulated models, and the "true" values considering blocks within a given distance from the boundary between  $Z_1$  and  $Z_2$ . The higher correlation coefficient with the true values shown by the blocks estimates from cosimulation indicate this model represent better the underlying correlation that exists between  $Z_1$  and  $Z_2$ .

The other comparison that was done considered the global variance of each realization calculated from blocks within a given distance from the boundary between  $Z_1$  and  $Z_2$ . As expected, the average of the global variance over all the realizations showed lower variance for the block values obtained using cosimulation instead of independent simulations (Fig. 8), and is closer to the global variance calculated from the same group of blocks in the 'true' reference map.



Fig. 8: Average global variance calculated from blocks within a given distance from the boundary between  $Z_1$  and  $Z_2$ . The average variance calculated from blocks estimated using cosimulation is closer to the global variance from the reference value.

### Conclusions

A significant step in mineral resource and ore reserve estimation is the choice of the geological domains as well as the type of boundaries between them. Geology should be used to define these domains. The geological mechanism to which the geological controls are due, are in most cases transitional in nature. This yields contacts between boundaries that are diffuse or gradational, and we should expect some degree of overlap between the estimation domains.

The estimation of a domain with a 'soft' boundary with any of its neighbors implies that samples from either side of the boundary should be used in the estimation. Nevertheless the samples outside from the domain should not be considered to follow the same distribution and spatial model as the samples inside, as they belong to distinct domains defined by different statistical parameters.

A linear model of coregionalization can be used to capture the spatial correlation of one variable across a boundary between domains. This spatial model is legitimate and allows for correct reproduction of representative statistics and the covariance model at locations near the boundary, where samples from both domains are used for the estimation of unknown locations.

The calculated LMC spatial model can be used in a full LMC cokriging or cosimulation to model a geological boundary using samples from adjacent boundaries. This alternative for the estimation of domains with 'soft' boundaries, as shown in the application, has the advantage of improved resource estimation by reducing the global uncertainty in transitional zones near the boundaries. It also shows a decrease of smoothing in the estimates if kriging is the tool to obtain the resources, and also the reproduction of data correlation across a boundary in the estimates, which can help for improved delineation of the mine plan.

The drawbacks of this methodology are the uncertainty associated with the determination of the nugget effect of the cross variogram, which will depend strongly on the number of data (grid spacing) available to characterize the contacts, and the shape of the contact surfaces relative to the spatial anisotropies of each domain. This uncertainty can have a big influence in the overall uncertainty of the final model. The extra time associated with fitting a linear model of coregionalization can be easily overcome by using semi-automatic fitting programs.

This methodology, assumes that the variable is stationary in each domain, and therefore can be used to model a **global** spatial relationship across a boundary. However, nature provides us with several examples, where the behavior of our variable of interest is no longer stationary as it gets closer to the boundary, such as an increase or decrease in the mean or variance near the boundary between two different geological domains. In this case we need to identify the non-stationary factors that affect the behavior of the variables near the boundaries, in the mean, variance and spatial covariance model in order to estimate or simulated using non-stationary kriging. A more detailed description of this new technique can be found in Larrondo and Deutsch (2004).

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