GEOSTATISTICAL UNCERTAINTY MODELING OF ACID ROCK DRAINAGE

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ABSTRACT

The estimation of actual or potential acid rock drainage (ARD) at mine sites is usually accomplished by sampling specific parameters that allow detection and prediction of the potential for ARD. The use of block models to estimate and describe the spatial extent of relevant variables is becoming more common, although quantification of the uncertainty associated with the problem is generally not available, yet it can be critical in an ARD characterization study.

Uncertainties in sampling and analytical processes, in the characterization of the volumes and areas affected or potentially affected by ARD, in the interpolation of sampled values, and in the characterization of physical processes that allow prediction of fate and transport, are always present. It is unrealistic to pretend that the estimation process is error-free, and thus it follows that it is important to provide adequate models of uncertainty, in addition to reasonable estimates of ARD potential. The model of uncertainty can then be used to develop technical risk assessments, including false positives or negatives of certain variables exceeding (or not) certain thresholds.

This paper outlines a stochastic method based on geostatistical conditional simulations that allows assessment and modeling of uncertainty in spatial modeling. This assessment is then translated into risk levels, allowing for a decision-making process that is based on levels of uncertainty. The concept of Loss Functions is illustrated with an example drawn from a porphyry Cu-Mo deposit in South America.
INTRODUCTION

Characterization of ARD is now a typical component of any Feasibility Study, remedial investigation, or closure planning in any mining project around the world, and requires a committed and time-consuming effort. This investment is orientated initially towards assessing the potential for ARD in the short and long term. Mitigation and minimization of future negative consequences of contamination on human population and ecosystem are also considered. The results of such mitigating effort are generally measured in terms of eco-health and, sometimes, human health risk assessment. During this process, assessment of the risk associated with estimation errors is almost always lacking.

ARD characterization is usually accomplished by gathering field data of different types, such as neutralization potential, total sulfide, sulfur (or rather, sulfate sulfur), carbonate and carbon dioxide, as well as water quality analyses and specific trace elements. Several authors have discussed the use of field samples and blocks models to characterize different aspects of ARD-related problems, see for example Miller and Hertel (1997), Downing and Giroux (1993), and Downing and Madeisky (1997).

Several factors contribute to technical risk, including but not limited to:

- Uncertainties in the initial sample collection, which are related to sampling techniques used, the specific locations that are sampled and not sampled (i.e., sample location biases), and the relationship between sampling methods and the heterogeneity of the elements being sampled. A common example is not sampling all the important rock or mineralogical types that may have an impact in ARD estimation and prediction.
- Errors related to sample preparation and analysis, see for example Gy (1982) and François-Bongarçon (1999), among others.
- Errors stemming from inadequate handling of data, including data entry and database management processes. These errors can be minimized using appropriate data handling and data quality objectives protocols.
- Limitations related to overly simplified or inappropriate data evaluation and modeling techniques, statistical analysis, etc. These include ignoring or overlooking significant sources of spatial and natural data variability.
- Measurement errors related to the concentrations of the variable being analyzed. In many instances, the acceptable contaminant levels are very close to their laboratory detection limits (MDLs). This may introduce a significant technical challenge at the time of sample analysis, since for most methods the accuracy and precision of the analysis degrades near the MDL. The concept of Practical Quantitation Limit (PQL) has been proposed to overcome this problem, see for example Gibbons (1994).
- Uncertainties related to the definition of the geologic domains or zones that control the distribution of the element or contaminants being analyzed.

Given the imprecise information handled, the overall uncertainty in the prediction processes involved may be significant. This uncertainty should be modeled, and should include uncertainties related to sampling and assaying, as well as geologic uncertainty and uncertainty associated with the spatial modeling of the variables.
METHOD

This paper proposes the use of geostatistical conditional simulations and the concept of Loss Functions to model the uncertainty involved in ARD assessments. These spatial stochastic simulation tools have become in recent years the preferred toolbox for uncertainty modeling and spatial data analysis for mining and petroleum applications.

Many of the statistical techniques sometimes used to analyze environmental data are based on stringent assumptions about statistical distributions, lack of spatial correlation, and independence among the samples considered. These are typical requirements of Gaussian-based statistical techniques often used, for example Analysis of Variance (ANOVA) and Cochran’s approximation to the Behrens-Fisher t-test, see among others Gibbons (1994), Gilbert (1987), and USEPA (1989). Therefore, these techniques are inadequate in spatial statistics, where correlation between different sampled points is known to exist.

Geostatistical Conditional Simulations

A general background of the theory of geostatistical conditional simulations is given in Goovaerts (1997) and in Journel (1988). The simulations are models that reproduce the full histogram and spatial continuity of the original conditioning data. Therefore, they honor the spatial characteristics of the spatial variable as represented by the three-dimensional sample data. In addition, it is possible to extend the use of these spatial statistical tools to the time dimension, see for example Rossi and Posa (1991).

By honoring the histogram, the model correctly represents the proportion of high and low values, the mean, the variance, and other spatial statistical characteristics of the data. By honoring the variogram it correctly portrays the spatial complexity of the variables, and the connectivity of low and high contaminant zones. These are fundamental variables that need to be considered in order to improve predictions and diminish predictive uncertainty. When several simulated images are obtained, then it can be said that a model of uncertainty has been obtained.

Conditional simulations are built on fine grids, as fine as possible given the hardware available, so that they correspond to approximately the support size of the original samples. The vertical resolution of the grid is a function of the support data, typically the size of the sampled or screened interval. Larger grid sizes may still be used sometimes because of the amount of computer time and hard disk space involved. In building a conditional simulation model, many of the decisions necessary in typical geostatistical estimations are required, most importantly regarding the definition of the simulation domains (stationarity). Changes in geologic or hydro-geologic domains require splitting the data into different populations. Boundaries between simulation domains can be hard (no data influence across the boundary) or soft, where some data is used from the neighboring domain. Thorough understanding of the behavior of extreme and outlier values in the sampled population is required. Issues such as limiting the maximum simulated grade should be carefully considered.

The simulation method itself should be decided based on the statistical characteristics of the variable being simulated, the quantity and quality of available samples, the availability of using
fuzzy information such as geologic descriptions, and the desired output. The most commonly used methods are the Sequential Gaussian (Isaaks, 1990) and Sequential Indicator (Alabert, 1986). The latter is more complicated, is based on multiple indicator kriging techniques (Journel, 1988), and requires the definition of several indicator cutoffs. The former is simpler and quicker, although more restrictive in its basic assumptions.

All available geologic and hydro-geologic information can and should be used, typically taking the form of “soft” or imprecise information. For example, statements such as “Rock type A is highly acid generating” can be used as prior probabilities in a Bayesian sense.

As with any geostatistical estimation exercise, variogram models should be obtained. These may be particularly problematic, since sometimes there are not enough field samples to obtain such models. This is a potentially serious issue, but there are a number of alternatives that can be resorted to when developing variogram models. Some of these include judiciously applying prior knowledge about the site, data censoring (or what to do with non-detects, sometimes a high proportion of the total sample population), allowed minimum and maximum data values, number of conditioning data to be used, search distances, and assumed directions of anisotropies.

When a number of these conditional simulations have been run and checked, then, for each point defined in the grid, there is a set of possible values for the simulated variable available. These values are interpreted to describe the model of uncertainty for that point, generally arranged as a posterior cumulative conditional probability curve. Preferably, a large number of simulations are needed to describe this curve better. However, due to practical limitations, a much smaller number, perhaps as small as 20-30 simulations, can be used as an initial approximation. When there is significant conditioning information, these simulated values for each cell will not vary much, meaning that the most likely value is known with a good degree of certainty. The opposite occurs when the cell has few samples nearby.

The model of uncertainty obtained for each point can be described as:

\[
F(z; x | (n)) = \Pr \{ Z(x) \leq z | (n), \alpha = 1,..., n \} \tag{1}
\]

\(F(z; x | (n))\) represents the cumulative conditional distribution frequency curve for each vector \(x\) of the simulated grid, obtained using the \((n)\) conditioning filed samples, and it provides the probability of that point in the grid of being above (or below) any contaminant value \(z\).

**Loss Functions**

Final recommendations in Feasibility Studies and Remedial Investigations (FS/RIs) are typically based on predicted impacts on ecosystems and/or health risk assessments, which in turn are based on estimates of contamination, \(z'(x)\). Since the true values at each location are not known, errors can and will likely occur. The loss function \(L(e)\) (Journel, 1988; Isaaks, 1990; Rossi, 1999) is a mathematical function that attaches an economical value (impact or loss) to each possible error, measured in, for example, dollars. If the full set of possible values is known at each location, for example in the form of the conditional probability distribution described in Equation (1), the loss function can be used to obtain the expected conditional loss:
The minimum expected loss is found by calculating the conditional expected loss for all possible values of the estimates, and retaining the estimate that minimizes the expected loss. As described in Isaaks (1990), the expected conditional loss is commonly a step function whose value depends on the assumed costs of each bad decision, and the relative of costs of miss-classification. This implies that the expected conditional loss depends only on the classification of the estimate \( z^* (x) \), not on the estimated value itself.

The Loss Function thus quantifies the consequences of false positives and false negatives, weighs the relative impact of each, the probability of each, and then derives the minimum cost solution. For example, in an operation where the mine plan contemplates using the acid neutralizing potential (ANP) of the in-situ rock to influence the scheduling of waste stockpiles, the loss incurred when rock is predicted to be high in ANP when in fact it is not is a direct function of the costs incurred. The cost of the mistakes made can usually be estimated and used to quantify risk. In some extreme cases, when a significant loss of health, quality of life, or life itself results, the cost can be assumed to be infinite. Figure 1 shows a typical Loss Function, where an overestimation error incurs in unnecessary costs, increasing linearly with the magnitude or the error, while an underestimation error causes the Loss to increase exponentially with the absolute value of the error, and for certain errors it becomes infinite.

\[
E \{ L (z - E) | (n) \} = \int_{-\infty}^{\infty} L(z - z^*) \cdot dF(z; x | (n))
\]

Figure 1: Hypothetical Loss Function.
An Example from a Large Open Pit Mine

The example described here corresponds to a large open pit porphyry Cu-Au deposit in South America. The purpose of the study was to evaluate the application of the geostatistical assessment of potential risks related to developing waste rock piles with nearly-zero net acid generating potential (AGP). Several variables have been analyzed from drill hole samples, including acid generating potential (AGP) and acid neutralizing potential (ANP) values, as well as sulfur in sulfates, pyrite, arsenic, etc. The information is obtained from blast holes, and is measured in kg/ton of H\textsubscript{2}SO\textsubscript{4}. This example is based on ANP, which is defined as the capacity for solutes plus particulates in an aqueous system to neutralize acid. It is an estimate of alkalinity, commonly measured in water samples, except that it is taken from non-filtered samples, i.e., includes the acid neutralizing capacity of the particulates that may be present. Therefore, it is deemed more representative of the overall acid neutralizing capacity of the in-situ rock.

The development of waste dumps with non-acid generating potential may be accomplished by alternatively stacking acid generating rock and rock with high ANP. A spatial estimate of both variables is required well in advance of mining, preferably at the time of preparing the life-of-mine plan, which in this case is about 15 years. In the case of this operation, it implies attempting to estimate in-situ ANP values no less than 200 or 300 meters below current surface.

A preliminary analysis of the data available showed that there are significant spatial and temporal variations in water quality in active and background wells, as well as in ex-pit surface water, and mostly dependent on seasonal rains. A conditional simulation (CS) model was developed covering the volume of the remaining mining reserves (within the designed ultimate pit) for ANP, ANC, S, and SO\textsubscript{4} using the Sequential Gaussian simulations (SGS) method. In order to develop the simulations, the following steps were completed:

1. Initial exploratory statistical data analysis was performed over the whole database. This included separating the ANP and other variables by domains, according to their geologic and statistical characteristics. Among those, there are three geological domains with significant amount of gypsum, which contributes significant amounts of SO\textsubscript{4}. These domains are located at the center and also towards the periphery of the deposit.
2. Variogram models were obtained for each variable within each domain. In some cases, due to data scarcity, only an omni-directional variogram was modeled. The models (not presented in this paper) showed significant spatial correlation within some units, with a relative nugget effect between 20 and 40% of total variance.
3. The simulation grid was defined on a 5 x 5 x 5m cell, and 30 simulations were obtained. These simulations provide the model of uncertainty of Equation (1). Figure 2 shows a plan view at level 330m of four of the 30 simulations representing acid-generating potential\textsuperscript{1}. Note that the general spatial trends are reproduced in all simulations; however, there are variations in the vicinity of higher values from simulation to simulation.
4. The simulations models were properly validated using the original data and all other simulations parameters chosen.

\textsuperscript{1} All values shown in this paper have been factored to protect confidentiality.
To visualize this model of uncertainty, multiple options are available. One possibility is to use probability maps, such as the one shown in Figure 3. In this case, the probability that the ANP variable be less than a critical threshold is shown\(^2\) for the same level 330m. Note that those areas with high probabilities are almost certainly acid-generating, while the most uncertain areas are those where probabilities are close to 50%, with little certainty one way or the other. The spatial trends observed are consistent with the known geology, including the structural, alteration, and lithology models, and also considering gypsum content, a significant provider of sulfates. Also, the high probability area to the southwest of the picture corresponds to a simulation domain with few drill holes, and requires further confirmation.

\[\text{Figure 2: Four simulated models, open-pit area, level 330m, Acid Neutralizing Potential.}\]

\(^2\) All thresholds used in this paper are not listed to protect confidentiality.
Developing the Loss Function

The Loss Function applied to evaluate risk in this case was based on the following Equation:

\[ \text{Loss} = \text{Actual Cost} - \text{Potential Cost} \quad (3) \]

The general expression for the costs associated with each type of error are depicted in Figure 1, where it is assumed that the costs of mishandling acid-generating rock increases exponentially with the error magnitude (which includes an unknown future liability), while the cost of neutralizing rock that did not needed to be neutralized increases linearly with the error magnitude. This is a conservative position to take because of the higher costs associated with not sufficiently neutralizing the waste rock in the dumps (false negative).

Applying a loss function similar to the one described, it is possible to find out the actual economic losses for each simulated value in each cell of the study area. Compositing these losses according to Equation (2) result in a mapped “optimal loss” classification. The loss map shown in Figure 4 is
based on the simulations and the specific economic conditions assumed. The unit shown is dollars per ton of material not properly neutralized. Note that, compared to Figure 3, the loss function suggests that, based on the false negative and false positive costs assumed, it is better to neutralize a larger volume of rock. The differences between both maps depend on how linear the loss function is. The associated risk for each type and level of error is not generally directly proportional to the probability of making the error, except when the loss function is linear for both error types. In this case, a probability measure from the conditional simulations (model of uncertainty) provides a direct measure of risk, which would make Figs. 3 and 4 similar.

**Figure 4: Loss function map, pit level 330m.**

**CONCLUSIONS**

When trying to model ARD-related variables, make decisions, and eventually operate and monitor a prevention or mitigation program, it is often difficult to accurately assess and predict a number of technical aspects of the problem. Most of these difficulties stem from intrinsic spatial and temporal rock quality variability, sampling inaccuracies, and methodological errors. These errors will lead to mistakes in the decision-making process and may have important consequences. A method has been proposed here whereby the modeled errors are incorporated into the technical risk evaluation
process through the use of stochastic conditional simulations, interpreted as models of uncertainty. This requires going beyond the use of block models as has been proposed in the past while attempting to not only estimate the values of relevant variables, but to also provide a model of uncertainty.

These models of uncertainty are then used to evaluate the consequences of all possible mistakes through the use of Loss Functions. Evidently, the quality of the final product will depend on the virtues of the model of uncertainty, and the accurate reflection of incurred additional costs through the Loss Function defined.

A major advantage of this method is its flexibility with respect to assessing costs, since in the formulation of the Loss Function there can be several types of costs included, such as the actual monitoring and mitigation operating costs, costs stemming from health risk assessments, other costs that would be more speculative, including socio-political costs. The cost of such flexibility is a more mathematically involved methodology, and the responsibility that results from actually explicitly stating the hidden assumptions that are inherent to any risk assessment process.

The end result should be a risk-based decision-making and planning performed on the basis of a sound modeling technique which incorporates key uncertainties associated with ARD prediction, as well as a quantification of the consequences of potential errors.

**REFERENCES**


