An Overview of Geostatistical Simulation for Quantifying Risk

by

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ABSTRACT

This paper presents an overview of geostatistical simulation with particular focus on aspects of importance to its application for quantification of risk in the mining industry. Geostatistical simulation is a spatial extension of the concept of Monte Carlo simulation. In addition to reproducing the data histogram, geostatistical simulations also honour the spatial variability of data, usually characterised by a variogram model. If the simulations also honour the data themselves, they are said to be 'conditional simulations'. In a sense, simulations are an attempt at 'sampling the unknown' using constraints, e.g. statistical moments imposed by the data. Thus, in simulation, the requirements of stationarity are stricter than for linear geostatistics (for example, kriging). Geostatistical simulation is much more computationally demanding than geostatistical estimation. However, the exponential increases in computer processing speed, memory and data storage capacity have brought these tools into wide operational use in the mining industry over the past decade. We can generate many (in theory an infinite number) of simulated images. The question still remains: 'how many simulated images are required to properly characterise a given domain?' To answer this we must test the simulations to ensure they reasonably reproduce the input statistics. The validity of any subsequent use of the simulations for risk characterisation will be heavily dependent on how well our set of simulations characterises the intended 'probability space'. There now exists a plethora of methods to generate simulations. The main methods in use in the mining industry today are discussed and we briefly introduce some less common approaches. Finally, the concepts of multivariate simulation ('co-simulation') are touched upon. In conclusion we summarise some of the uses of geostatistical simulations for application to risk quantification problems in the mining industry.

Key Words: *conditional simulation; stochastic simulation; geostatistics; risk analysis; confidence interval; Monte Carlo simulation; turning bands simulation; sequential Gaussian simulation; sequential indicator simulation; p-field simulation; LU decomposition; pluriGaussian simulation; truncated Gaussian simulation; Object-based simulation; Frequency-domain simulation; simulated annealing; variogram; histogram; stationarity; conditional co-simulation; pit optimisation; grade control; resource estimation; kriging.*

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INTRODUCTION

This paper presents an overview of geostatistical simulation with a particular focus on aspects of importance to its application for quantification of risk in the mining industry, although touching on some other application areas. We deal here mainly with univariate simulation, that is, simulation of a single variable, however, we also briefly introduce the concepts of multivariate simulation ('co-simulation').

This is a review paper intending to summarise the broad field of geostatistical conditional simulation. As such, an extensive bibliography is given. This bibliography goes beyond the papers cited in the text of our paper and is intended to give readers an entry to the primary literature. A good, modern overview of simulation is given by Chiles and Delfiner (1999). An excellent mathematically rigorous summary of algorithms is given by Lantuejoul (2001).

CONCEPTS

MOTIVATIONS

Good estimation has the goal of providing the 'best' estimate for a block. This is achieved in kriging by reducing the estimation variance to a minimum for all possible linear weighted averaging schemes. This is a good argument to use kriging if mapping local 'in-situ' averages is the key issue.

However, if we wish to deal with issues of variability, kriging has a downside. The means of achieving minimum estimation variance in kriging is to smooth the values. This is a consequence of the 'information effect' (Journel and Huijbregts, 1978) and implies that the estimated block values have a lower variance than the 'true block' values. Such smoothing is necessary to minimise conditional bias.

Making the blocks smaller results in the unrealistic smoothness of the blocks getting worse (see extensive bibliography warning about 'small block kriging' listed in Vann and Guibal, 2000).

WHAT IS SIMULATION?

Venikov (1969) defines simulation as:

"…a system of models … having a definite resemblance to the first system (the original)."

The word 'model' is derived from the Latin 'modus', meaning 'measure' or 'image'. In geostatistics we produce such models to represent the spatial distribution of variables. These models – or images – are a class of scientific model and thus should have properties that reflect attributes of the reality we are attempting to model.

MONTE CARLO SIMULATION

Monte Carlo simulation is at the heart of geostatistical simulation. In essence, a Monte Carlo simulation generates a 'realisation' of a random process. A random process might be described by a histogram ('distribution') and a variogram or covariance (describing time-domain or spatial autocorrelation). By drawing values sequentially from a histogram we can generate a possible sequence of values that is consistent with that histogram. Rules can then be applied to ensure that the variogram (or other correlation measure) is also reproduced. As a simple example, we might draw random values from a (very simple) histogram showing 50% of outcomes as 1 and 50% as 0. We will impose no autocorrelation (that is the variogram is implicitly 'pure nugget'). The result is a Monte Carlo Simulation of a binary process with equally likely outcomes: tossing a coin!

GEOSTATISTICAL SIMULATIONS

A key property of geostatistical simulation models (as opposed to geostatistical estimation, or kriging, models) is that a *family or system* of model realisations is generated, i.e. not one 'best estimate'. We produce a series of images, or 'realisations', that presents a range of plausible possibilities. The plausibility of these possible images is dependent on the assumptions and methodology employed in the simulation process.

Conditional simulation (CS) builds many such realisations of mineralisation, each reproducing the histogram and variogram of the input data, as well as honouring the known data points (hence 'conditional'). There is a clear distinction between methods where conditioning is in-built, e.g. so-called 'sequential methods' and those where conditioning takes place as a separate kriging step (e.g. turning bands).

Each realisation is different to others because we always have uncertainty away from known data points (drill samples); hence individually such realisations are 'simulations' not estimates.

Simulation has different objectives to estimation. The whole point is to reproduce the variance of the input data, both in a univariate sense (via. the histogram) and spatially (through the variogram or other covariance model). Thus simulations provide an appropriate platform to study any problem relating to variability, for example risk analysis, in a way that estimates cannot.

At point level estimates honour the known data (this is a property of point kriging), but they don't reflect the variability *between* points – because of necessary smoothing. To contrast to this, a simulation has the same 'character' as the true profile: the histogram and variogram of a simulation are in agreement with those of the data.

PROPERTIES

There are theoretically an infinite number of simulations that can meet the above conditions. This set or family of simulations are often referred to as 'equiprobable images' of the mineralisation (which has the same meaning as 'realisations', in the sense that they are drawn at random from a specified spatial distribution). Although conditional simulations are customarily described as 'equally likely' (or 'equiprobable') images of the mineralisation, this is not strictly mathematically true. For example, gold deposits usually have positively skewed distributions. This implies that a tail of low frequency high grades exists, but these grades carry disproportionate metal (thus profit). When we simulate we generate values that more or less follow the input distribution. However, the exact histogram is not reproduced. As a consequence, *some images have slightly more high grades and some slightly fewer.* This is the reason that we can rank images as 'optimistic', 'median' or 'pessimistic'.

Any individual simulation is a poorer estimate than kriging. However, averaging a set of simulations can yield a good estimate. A collection of many such simulations, when averaged over a block volume, is equivalent to a kriged estimate.

Because we can have multiple realisations within each estimated block, in mining applications we can have access to the *local distribution* of metal within a block – as for Uniform Conditioning (UC), Multiple Indicator Kriging (MIK) or any other non-linear geostatistical estimate of recoverable resources. Thus CS is a potential route to recoverable resource estimation (see Vann and Guibal, 2000, for a summary of recoverable resource estimation).

In a sense, simulations are an attempt at 'sampling the unknown' using constraints, e.g. statistical moments imposed by the data. Thus, in simulation, the requirements of stationarity are stricter than for linear geostatistics (for example, kriging).

So, we can generate many simulated images. The question still remains: 'how many simulated images are required to properly characterise a given domain?' To answer this we must test the simulations to ensure they reasonably reproduce the input statistics. The validity of any subsequent use of the simulations for risk characterisation will be heavily dependent on how well our set of simulations characterises the intended 'probability space'.

MAIN APPROACHES TO SIMULATION

Simulation methods are highly dependent upon the nature of the variable to be simulated (i.e. the problem at hand). Three classes of variables can be distinguished:

1. Continuous variables that usually represent physical properties (e.g. mineral grade, layer thickness);
2. Categorical variables (eg. lithofacies, geological units, grade envelopes); and
3. Objects that are defined by their location, shape and orientation (e.g.

sedimentary channels, mineral grains).

Depending on the choice of the variable, some methods will be more suited to reproducing the spatial distribution. In particular, geostatistical simulation methods depend on the choice of a model for the distribution of the variables of interest, partly characterised by the histogram and the variogram. The model chosen can be used as a basis for classifying simulation approaches. The classification employed here is based on the underlying geostatistical models used for different simulation methods but does not pretend to be exhaustive (for more details see Chiles and Delfiner, 1999).

PIXEL-BASED METHODS

This class of methods are based on the definition of an array of pixels or points (usually in the form of a regular grid) to which a certain characteristic is attached. To date, most applications of geostatistical simulation, especially for risk characterisation in mining problems, have employed pixel-based methods.

Non-parametric methods

Generally, these methods are a product of the indicator approach to geostatistics (see Journel, 1982, 1983, 1987, 1988, 1989; and Journel and Alabert, 1989). The two most frequently applied non-parametric methods, sequential indicator simulation (SIS, see Gomez-Hernandez and Srivastava, 1990) and p-field simulation (Srivastava, 1992; Froidevaux, 1993), are discussed in this paper.

Gaussian-based methods

These methods rely on Gaussian random functions (the 'multiGaussian approach', see Goovaerts, 1997) and presume the 'diffusion' model[2] (for more details on diffusion models and alternatives, see Rivoirard, 1994; and Vann et al., 2000). The diffusion model is consistent with mineral deposits exhibiting gradational grade transitions: from high grade cores towards the outer rings of lower grade material (at various scales, and not necessarily as a simple 'bullseye'). In mining situations, the authors have observed that the diffusion model applies to many deposit types, including porphyry Cu-Au and some types of Archaean Au systems.

The two main methods in this class, widely applied in mining risk analysis, are the turning bands (TB) and sequential Gaussian simulation (SGS). More details of these are given later. Other Gaussian-related techniques include truncated Gaussian and pluriGaussian (Armstrong et al., 2000).

Fractals

The 'fractal dimension' of a spatial distribution can be modelled using a power semi-variogram in such a way that the fractal nature of the distribution is maintained when the original distribution is simulated (see Kentwell and Bloom, 1998). Fractal methods are not widely used in the mining industry. The limitation of the acceptable variogram models to the power model is probably one of the main reasons for their restricted use.

OBJECT-BASED METHODS

Point processes

Point processes involve spatial realisations of pre-defined distributions (e.g. Poisson or Cox processes). They can be used to model a wide range of phenomena (eg. distribution of trees in forests, or gems in precious stone deposits). They also offer the flexibility of being able to be used as components of more complex models (eg. Boolean methods). For an example of this approach applied to precious stones, see Kleingeld et al. (1997).

Boolean methods

Random sets can be constructed by locating independent random objects, the shapes and orientations of which are drawn from pre-defined statistical distribution, at Poisson points. These models have found favour with

[2] Also referred to variously as the 'diffusive', 'edge-effect' or 'border-effect' model

petroleum geologists who appreciate the geological 'flavour' of the reconstructed reservoir architecture. However, the statistical inference of the model is not straightforward.

NON-PARAMETRIC METHODS

SEQUENTIAL INDICATOR SIMULATION (SIS)

The use of indicators is a strategy for performing structural analysis appropriate for characterising the spatial distribution of grades at different cut-offs, or categorical variables. Indicator simulation approaches now have a long history: see Alabert (1987); Chu (1996); Gomez-Hernandez and Cassiraga (1994); Gomez-Hernandez and Srivastava (1990); Isaaks (1984); Journel and Alabert (1989); and Journel and Isaaks (1984).

Sequential indicator simulation (SIS) was developed for application in petroleum reservoir modelling where extreme values (high permeabilities) are well connected in space. This high connectivity of extreme values is difficult to model in the multigaussian paradigm. Another major advantage of the SIS algorithm is that hard data and soft data can be easily mixed. SIS is a very efficient algorithm.

The algorithm is as follows: After defining a random path through the nodes to be simulated,

- Discretise the distribution into (k+1) classes using k thresholds (or cut-offs).
- Transform the data to a vector of indicators (1 or 0) depending on exceedence or not of the thresholds.
- Determine k ccdf (conditional cumulative distribution function) values using an indicator kriging algorithm.
- Correct for order relations (see further below). Then build a complete ccdf model.
- Draw a simulation value from that ccdf.
- Add the simulated value to the conditioning data set.
- Proceed to the next node on the random path and repeat the above steps.

DRAWBACKS OF SIS

A main difficulty with SIS is as for multiple indicator kriging (MIK), i.e. order relation problems (Vann and Guibal, 2000; Vann et al., 2000). Because indicator variogram models may be inconsistent from one cut-off to another we may predict from SIS more recovered metal above a cut-off Z_{C2} than for a lower cut-off Z_{C1}, where $Z_{C1}<Z_{C2}$, which is clearly impossible in nature. There can be quite severe difficulties in this regard with MIK, and the same type of problem can be observed with SIS.

While 'order relation corrections' are usually programmed, these do not fix the underlying problem: the theoretical solution is to account for the cross-correlation of indicators at different cut-offs (i.e. co-simulation of indicators), but this is completely impractical from a computational and time point of view.

A further drawback is that the quality of the simulation is sensitive to the kriging neighbourhood employed (often too small).

P-FIELD SIMULATION

The p-field algorithm consists of two main steps:

- establishing a set of local probability distributions; and
- repeated Monte Carlo simulation from these distributions with correlated probability values.

A wide variety of methods can be used to establish the local distributions, including multiGaussian and indicator approaches. P-field simulation is very efficient and conceptually simple. Note that there is a theoretical link between p-field, truncated Gaussian and sequential Gaussian methods (Journel and Ying, 2001).

Srivastava (1992) presents a petroleum application and Goovaerts (1997) gives more theoretical detail. Khosrowshahi and Shaw (1997) and Khosrowshahi, Gaze and Shaw (1998) give mining applications.

DRAWBACKS OF P-FIELD SIMULATION

P-field simulation suffer two main drawbacks which can be extremely detrimental (especially in a mining context):

- nodes close to the conditioning data commonly appear as local minima or maxima of the simulated realisations (this was identified first by Srivastava, 1992); and
- the simulated values usually show greater continuity than the original data.

Pyrcz and Deutsch (2001) detail these problems, coming the conclusion that the two flaws identified above are inherent in the algorithm. These authors recommend that p-field simulation not be used.

GAUSSIAN-BASED METHODS

GAUSSIAN TRANSFORMATION

All Gaussian-based methods rely on raw data being transformed to have a Gaussian distribution. A Gaussian transform (or 'anamorphosis') is a simple technique whereby a raw data population is transformed to have a normal (Gaussian) distribution with zero mean and unit variance. For each raw data value a Gaussian equivalent is generated via the cumulative histograms for both the raw and Gaussian distributions.

Gaussian distributions can then be transformed back to raw space via numerous methods. The two common approaches are by a simple graphical method or a more complex but more mathematically useful technique using Hermite polynomials (Marechal, 1978; Riviorard, 1994).

SOME COMMENTS ABOUT MULTIGAUSSIANITY

For all Gaussian random functions, the hypothesis is that the Gaussian distributed values are multiGaussian (as a consequence *all* bi-variate regressions are linear, however this property is necessary but not sufficient for multiGaussianity). Whilst multiGaussianity is practically impossible to prove, there are checks that can be made for biGaussianity. These involve calculating variograms on the Gaussian data and indicator variograms of the same and comparing graphically (see Goovaerts, 1997). Whilst demonstrating biGaussianity does not prove multiGaussianity, failing to demonstrate biGaussianity suggests you should try another method.

TURNING BANDS SIMULATION

Turning Bands (TB) was the first large-scale 3D Gaussian simulation algorithm implemented (Journel, 1974, Mantoglou and Wilson, 1982). The method works by simulating one-dimensional processes on lines regularly spaced in 3D. The one-dimensional simulations are then projected onto the spatial coordinates and averaged to give the required 3D simulated value. The method is very efficient for generating non-conditional simulations and particularly good at replicating the variogram. Conditioning is obtained through a separate kriging step:

- Non-conditional simulations at all target points and all sample points ($Z_s(x)$)
- Krige values to all sample points using real data ($Z_K(x)$)
- Krige simulated values at all points ($Z_{KS}(x)$)
- Combine using $Z_{CS}(x) = Z_K(x) + [Z_s(x) - Z_{KS}(x)]$

A main advantage of TB is that it reproduces the variogram better than other methods for small simulated fields (e.g. grade control applications).

DRAWBACKS OF TURNING BANDS SIMULATION

The Turning Bands method used to suffer two 'mechanical' limitations:

- In 3D, the maximum number of lines regularly distributed in space was limited and the simulations sometimes showed "banding" effects which are unrealistic.
- Only certain specific variogram models (including the spherical and the exponential models) could be simulated.

The second limitation is irrelevant in mining applications, as it is practically always possible to model experimental variograms using combinations of elementary spherical and/or exponential functions.

The first limitation has been effectively eliminated since it has become possible to use as many bands as possible (e.g. 3-400) although TB is still considerably slower than sequential methods.

Other limitations of TB are related to the assumptions of multiGaussianity (as for SGS, below).

SEQUENTIAL GAUSSIAN SIMULATION (AND VARIANTS)

The Sequential Gaussian simulation is an efficient method widely used in the mining industry. The algorithm, in very simple terms, defines a random path through all grid nodes (including the conditioning samples). Simple kriging of the nodes in the path helps generating a local distribution. A new value is then drawn from this local distribution. This added to the nodes in the random path and the next node is simulated (and so on).

The actual algorithm is as follows:

- Define a random path through all grid nodes
- To simulate the first grid node given the n conditioning data (taken out of a neighbourhood centred on the target node), estimate its value by simple kriging - y_1^*. Then select a Gaussian residual R_1 that is independent of y_1^* and calculate $y_1 = y_1^* + \sigma_{SK} R_1$ (which is the local conditional expectation in the multiGaussian model).
- Add the new value y_1 to the conditioning data set.
- Draw a value y_2 from the conditioning distribution of the random variable Y_2 at the second grid node given the (n+1) conditioning data: again a simple kriging is required.
- Repeat until all nodes are simulated.

DRAWBACKS OF SEQUENTIAL GAUSSIAN SIMULATION

For all Gaussian methods the size of the field being simulated must be much larger than the range of the variograms (this is also true for turning bands).

For SGS, (as for SIS) the biggest problem is the search neighbourhood selection. The selection of small neighbourhoods can lead to poor conditioning and poor replication of the variogram.

OTHER GAUSSIAN SIMULATION METHODS

Truncated Gaussian is a method that is used for simulating sequentially ordered lithofacies by truncating a multiGaussian random function *Y(x)* (Galli et al., 1994). Once the covariance of *Y(x)* has been determined, the simulation of *Y(x)* can be performed using a sequential algorithm.

These techniques are well suited to petroleum reservoir simulation. They also have possible applications in mining for grade simulation when the grade distribution is highly correlated to lithotype and shows different spatial characteristics for different units.

NUMERICAL RECIPES

There are numerous numerical recipes for generating independent processes with a given covariance (see Lantuejoul, 2001). We briefly touch upon the main techniques used to generate multiGaussian processes and describe some different well-established techniques.

LU DECOMPOSITION

A very important category consists of the algorithms used to generate Gaussian spatial processes. One can generate a sequence of Gaussian variables with a given covariance by evaluating the square root of the covariance matrix. Various decomposition methods exist; the most frequently used being the LU (Choleski) decomposition (see Davis, 1987; Davis and Wilkins, 1991). These methods suffer from efficiency limitations related to the size of the matrices to be handled. There are essentially used for small simulations.

FREQUENCY-DOMAIN APPROACH

Frequency domain approaches are also common. Here the covariance is reproduced through sampling of its discretised Fourier Transform. We then use the inverse Fourier Transform to obtain the realisation of a discrete spatial process.

SIMULATED ANNEALING

Simulated Annealing has gained ground over the past decade, especially in the petroleum industry (Deutsch and Cockerham, 1994; Goovaerts, 1996). Starting form an initial image, where only the histogram is reproduced, nodes are swapped in pairs, the swap being accepted if a pre-specified objective function is lowered. The simulation stops when no swap lowers the objective function. The image must be cooled slowly (hence 'annealed') in order to avoid local minima.

MULTIVARIATE SIMULATION

Conditional simulation, as outlined above, deals with a single variable. Conditional co-simulation (CCS) is conditional simulation of more than one variable. The area of multivariate simulation is a fertile one for mining applications. We refer the reader to Carr and Myers (1985), Goovaerts (1997), Verly (1993) and Wackernagel and Grzebyk (1994).

We can imagine simulating more than one variable (e.g. gold and copper in a porphyry, grade and contaminants in an iron orebody; multivariate trace elements in geochemistry or environmental science, etc.). If we perform independent simulation of our multivariate set, the resulting simulations will not reproduce the correlation between these variables.

A simulation technique that overlooks the modelling of 'cross-structures', seen in cross-variograms, would miss the crux of the problem in some situations. For example, univariate recoverable resource estimation. Most univariate approaches can be generalised to multivariate application.

USE OF GEOSTATISTICAL SIMULATIONS TO CHARACTERISE RISK

Each simulation provides an alternative equiprobable representation of the distribution (or for CCS, the joint-distribution) of variables, meaning that we can get as many equally realistic answers to any of our questions as we want. The differences between these answers give us a measure of the joint spatial uncertainty and can help us manage the financial risk attached to the project.

CONFIDENCE INTERVALS AND RISK

It is difficult to associate a confidence interval to an estimate and it is well known that the ordinary kriging variance does *not* allow the construction of such an interval, except under specific circumstances (Gaussian distribution of errors) that are probably never met in practice. In fact, the kriging variance, like the kriging weights, does not depend on the data values themselves, and we expect a confidence interval to be heavily dependant on the values: in a positively skewed distribution, high values are less likely than low ones, thus the confidence intervals will be wider and the risk higher.

Simulations can be used to build confidence intervals empirically: many different simulations of a variable being calculated, we have access, at each point, to a complete empirical distribution (histogram); we are thus able to evaluate the probability for a given variable to take a value belonging to a given interval. This is precisely the notion of a confidence interval.

RISK ANALYSIS IN MINING

Consider open pit optimisation as an example: In general, such optimisation is carried out on a single model, say a kriged (or other estimated) estimated block model. The optimisation program implicitly assumes that all the blocks are estimated equally reliably (i.e. it treats them the same way). This is virtually never the case, for example, the density of drilling data decreases with depth.

An alternative is to build a large set of simulations (say 50, 100 or more) and to run the pit optimiser on representative members of the set: say, at least, the "worst" (10^{th}

percentile?), "median" (50th percentile?) and "best" (90th percentile) cases. We could select a much larger number of simulations (N being limited by computer resources only) and the outcome of the optimisation would then be not *one* net present value (NPV), but a *distribution* of NPV's allowing us to better quantify the risk involved.

The simulation approach would also take into account the differences in reliability between block grades: a block located in a badly informed zone will vary widely from one simulation to another, whereas blocks located in well drilled areas will vary little, due to the conditioning effect.

This approach can be extended to shorter term mining problems and grade control applications. Various mining schedules can be tested on one or several different simulations.

In general, conditional simulations are ideal inputs for studying the technical and economic effects of complex mining operations; for instance, multivariate optimisation problems, complex geometries in underground mining, etc.

CONCLUSIONS & RECOMMENDATIONS

The discipline of geostatistics is now nearly 40 years old, and it is 30 years since the first conditional simulation algorithm was developed (Journel, 1974). There are now a large (and ever increasing) number of operational conditional simulation tools to choose from. Understanding the underlying assumptions and mathematics of these methods is critical to making informed choices when selecting a technique for a specific application, for example risk-characterisation.

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