Advanced Methods

This section presents an overview of advanced geospatial methods, which are used to estimate values at unsampled locations and model the spatial correlation of the data. These methods include varieties of kriging and conditional simulation. Kriging is a spatial interpolation method that allows estimation of values at unsampled locations and provides an estimate of the uncertainty in the interpolated values. Selection of a particular kriging method depends on the characteristics of the data set, such as trends present in the data or the degree of spatial correlation, which can be determined using variograms and other spatial correlation models. Information about using spatial correlation models, different kriging methods, and conditional simulation is also presented in this section.

Spatial Correlation Models for Advanced Methods

Kriging and simulation methods require a model of spatial correlation. Spatial autocorrelation can be modeled using the variogram or covariance function. Typically, the empirical variogram is plotted based on the data, and a variogram model is fit to the empirical variogram. These activities may be referred to as variography. In general, variography encompasses directional spatial autocorrelation, bivariate autocorrelation, and multivariate spatial autocorrelation.

Most advanced geospatial methods rely on a search neighborhood to generate spatial predictions. The search neighborhood is selected based on the underlying spatial autocorrelation in the sampled population, and is simply the radius within which known values are used to predict unknown variables. Recognizing that correlation decreases with distance, the optimal search neighborhood is one which includes known values with a large influence and excludes the rest.

Construction of the Empirical Variogram

As part of EDA, the empirical variogram is constructed by plotting one-half the squared difference in values (semivariance) for each pair of sampling points as a function of distance separating the points (variogram cloud; see Figure 78). The variogram expresses the variability of the data set as a function of space: if data are spatially correlated, then on average, close sample points are more alike and have a smaller semivariance than samples farther apart.

The choice of the variogram parameters (for example, lag, direction) is a fundamental step for using advanced geospatial methods and should be done so as to be as representative as possible of the spatial characteristics of the data set. For example, if anisotropy is observed, which is common in environmental data, then an anisotropic variogram must be built that takes into account different spatial directions. Experimental variogram parameters are intrinsically linked to each particular data set; nevertheless, some recommendations can be made in order to create a suitable experimental curve.

Lag

When sampling is performed by following a regular grid, the regular distance between samples is taken as the value of the variogram lag. Distance between samples, however, is often irregular and the lag of the variogram then may be chosen by taking into account the different distances between the pairs of sampling locations. In this case, the value of the lag may be calculated by taking the average of distances between the sampling locations. As the distance between samples becomes larger, the reliability of the estimates of semivariance goes down. Consequently, a rough rule of thumb is that the maximum lag distance should not exceed half of the maximum distance between samples (see Figure 76).

▼*Read more*

Usually expressed as a percentage, lag tolerance corresponds to how much the distance between sample pairs can differ from the exact lag distance and still be included in the lag calculations. Tolerance of 0.5 or 50% is usually chosen for the calculation of the lag tolerance.

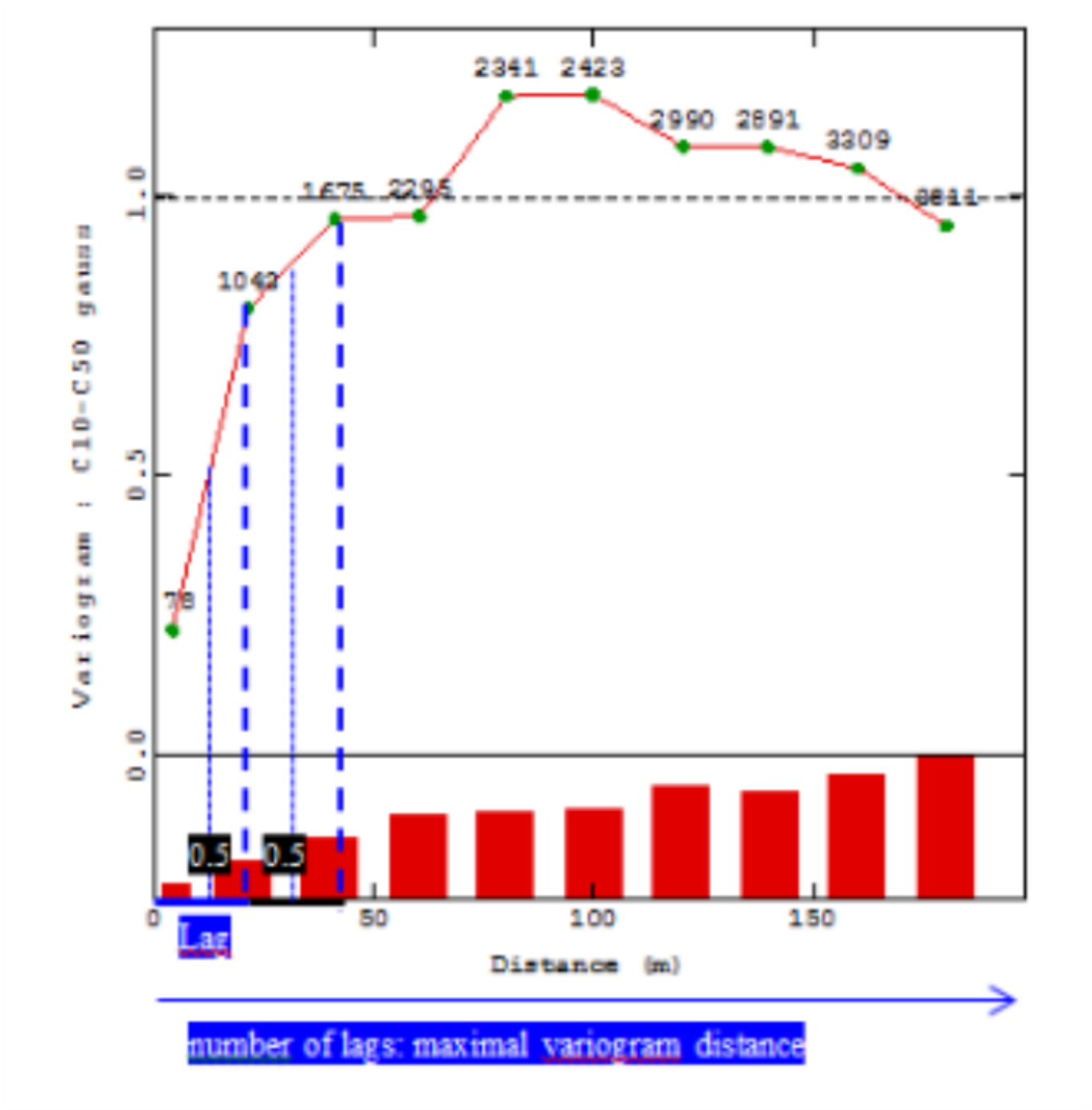


Figure 76. Example of an isotropic variogram; lag = 20 m; tolerance lag = 0.5, using Isatis.

Angle

Environmental data often has different levels of spatial correlation in different directions, which is referred to as anistropy. It is essential to account for anisotropy in variograms. Generally, the variogram map is used as a visualization tool for identifying anisotropic behaviors (see Figure 77). Anisotropy can be quantified by examining variograms constructed from data pairs along different directions. For example, it is possible to build a variogram by dividing the plane into four equal parts of 45°. Then, four variograms are constructed: one for the direction where the maximum spatial correlation is observed (reference direction) and three other perpendicular directions in order to define the lower levels of correlation in other directions. It is also possible to calculate the short-range variogram by taking shorter lags in order to specify the behavior at the origin.

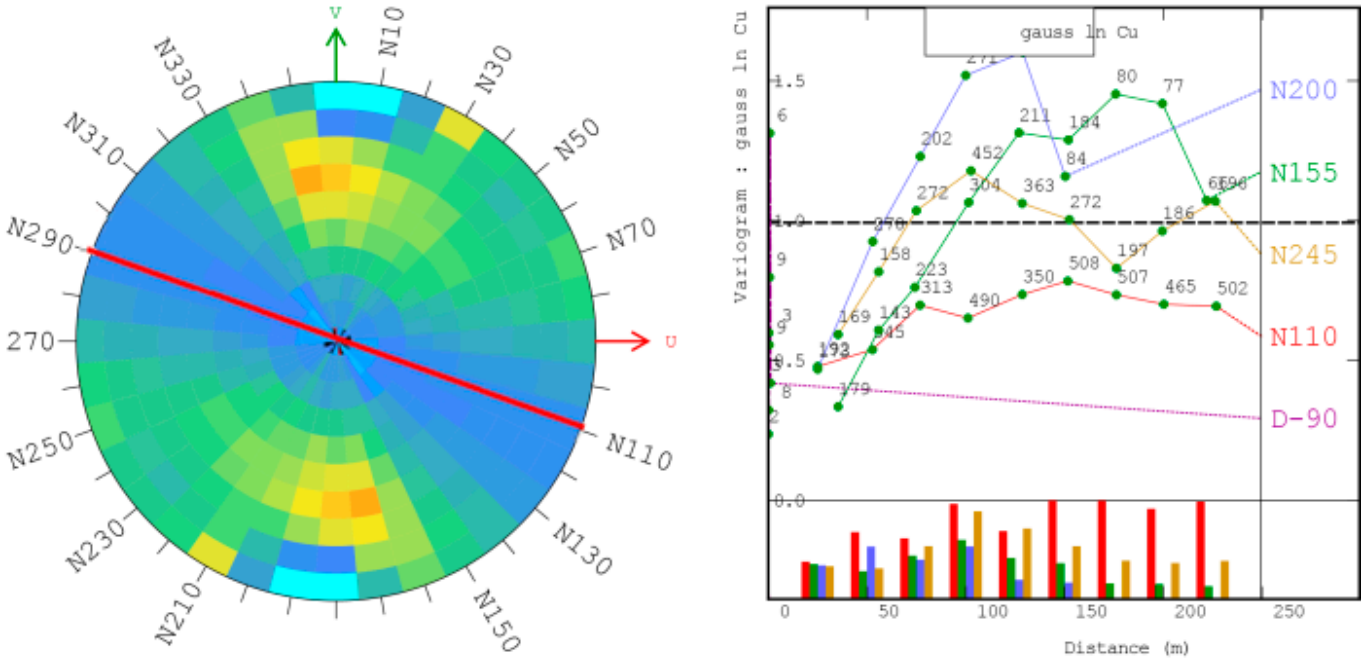


Figure 77. Example of an anisotropic variogram taking into account the anisotropic direction (N110°) as reference, using Isatis.

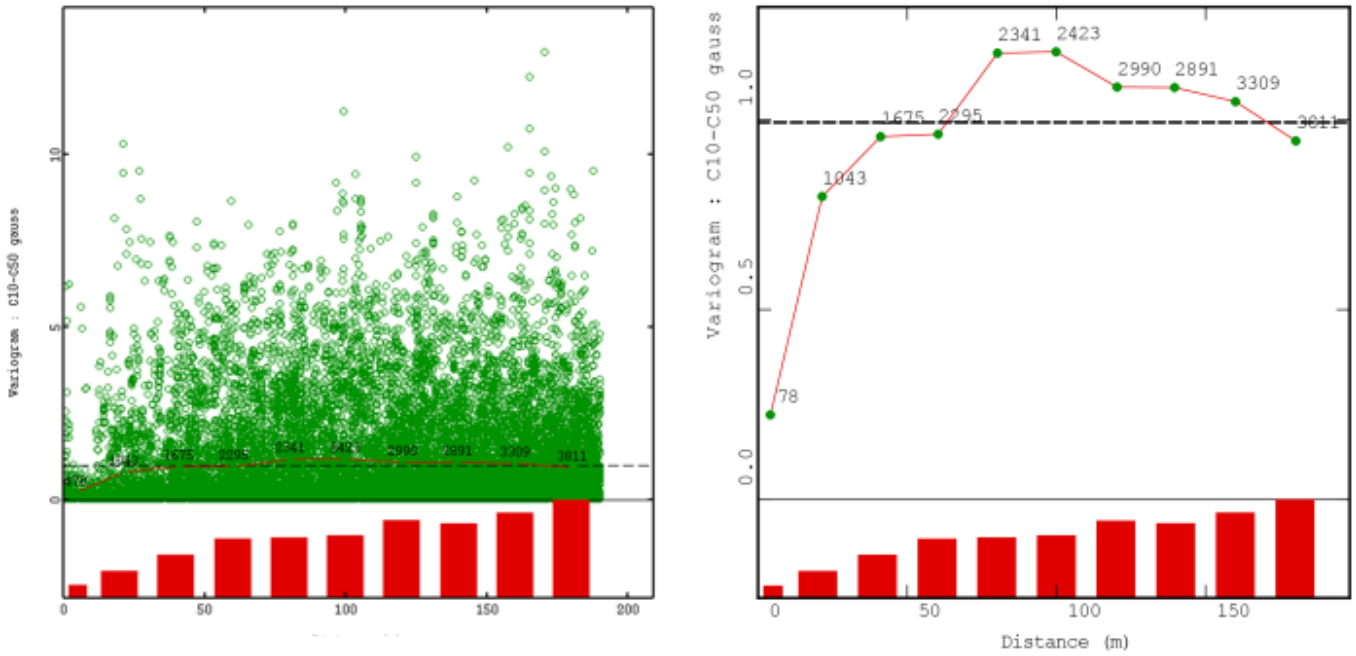


Figure 78. Variogram cloud (left) and experimental variogram (isotropic, log value = 20 m) (right), using Isatis.

Fitting the Empirical Variogram

The fitting model chosen is used to calculate the data values (for example, contaminant concentrations) at each modeled point. Therefore, a model must be created that is as representative as possible of the data and, by extension, of the experimental variogram previously constructed. The data set characteristics can guide the choice of the model to be used.

▼*Read more*

For example, if contaminant concentration varies rapidly, the initial gradient of the empirical variogram will be steep. In this case, an exponential or linear variogram may better represent this behavior. If a noncontinuous behavior is expected (inorganic contamination, for instance) or if analytical or sampling error is suspected, the nugget effect may represent such uncertainties.

Theoretical variogram models commonly used include exponential, spherical, Gaussian, Matérn, and linear. With the exception of the linear model, these theoretical models differ primarily in their behavior close to the origin. An illustration of the common theoretical variogram models is shown in Figure 79.

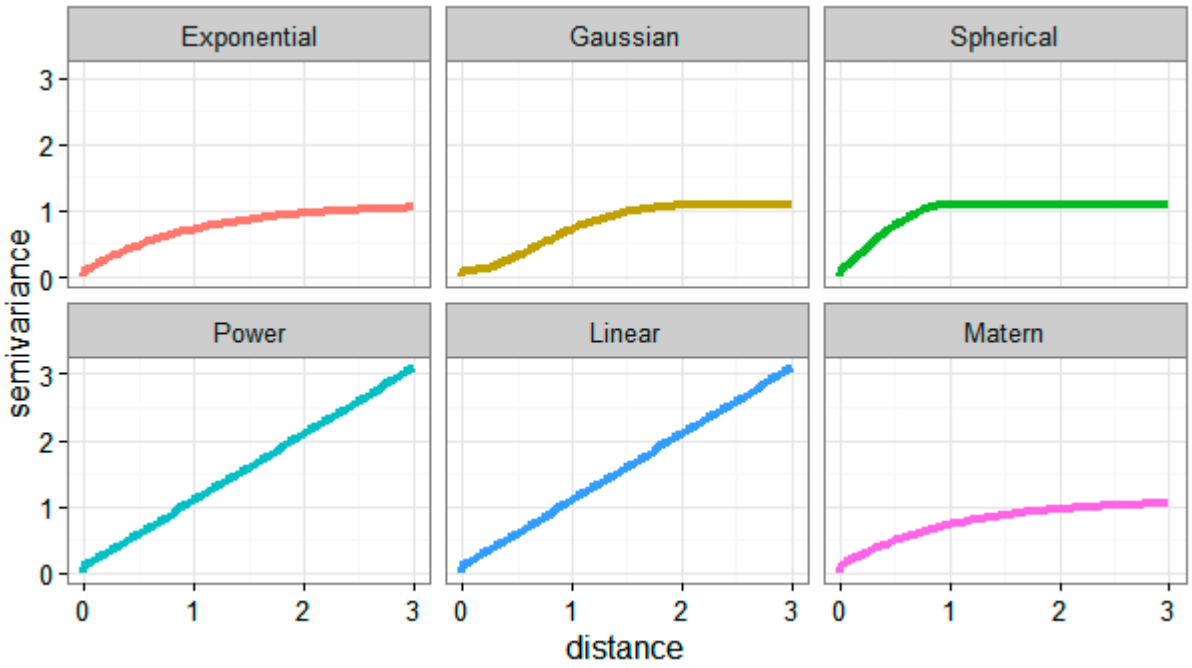
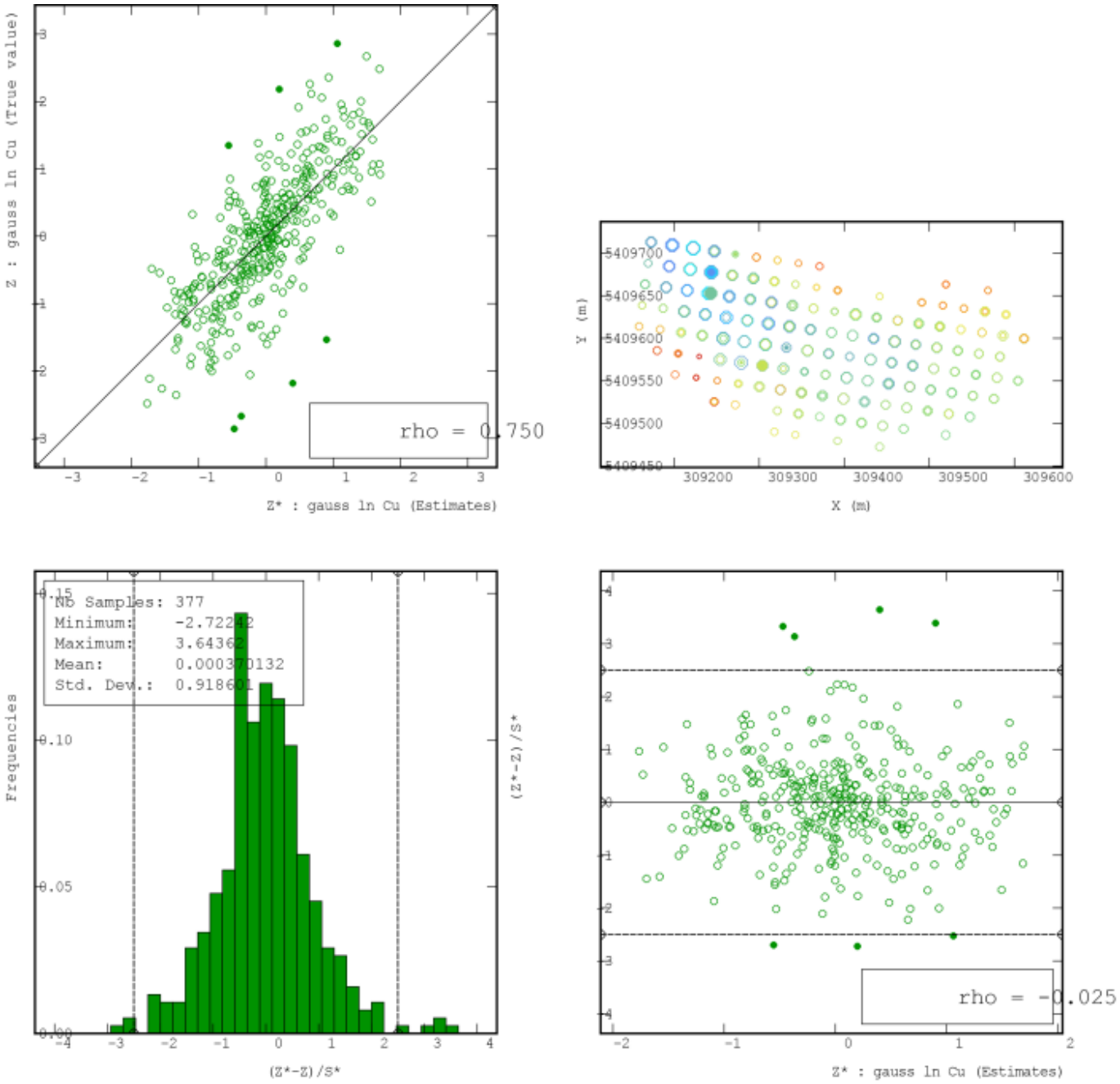


Figure 79. Theoretical variogram models.

When fitting a variogram, whether to use a nugget effect, and the most suitable range or sill value must be determined. It is best to produce several variogram models that could match with the contaminant concentration behavior. Then, cross validation can be used to compare the accuracy of each model in order to identify the most appropriate.

In the cross-validation process, several errors can be calculated (such as mean standardized error or mean error). A robust model shows a standard error of the variance close to 1, a strong correlation between the true values and the estimated values and, finally, a standard error close to 0. Through the analysis of these parameters, the most suitable model (the most accurate) can be chosen. Figure 80 illustrates a cross-validation example and error analysis.



MODEL	XVAL GAUSS	XVAL RAW	CONSISTENT DATA	Error Mean	Error variance	Std Error Mean	Std Error Variance
Anisotropic(NO-D90) with nugget	0.750	0.760	370	-0.01036	0.34982	-0.01462	0.67919
Anisotropic (NO-D90) without nugget	0.738	0.747	373	-0.02542	0.39154	-0.02920	0.50593
Anisotropic (NO)	0.718	0.732	371	-0.01333	0.39511	-0.01811	0.60920
Isotropic NO-D90	0.762	0.771	356	-0.00104	0.26511	-0.00274	1.01035
Omnidirectional with nugget	0.635	0.652	344	-0.05991	0.29000	-0.12343	1.05749
Omnidirectional without nugget	0.677	0.669	134	0.01905	0.02678	0.03953	1.88664

Figure 80. Cross-validation example and error analysis using Isatis.

Kriging

Kriging often relies on an optimal search neighborhood to generate spatial predictions. The optimal search neighborhood is determined by the underlying spatial autocorrelation in the sampled population. In general, kriging uses sampled values, within a pre-defined search neighborhood (defining the maximum and minimum number of "neighbors" to use), to estimate values at unsampled locations with a measured degree of confidence (called the kriging variance). The search neighborhood is optimized through evaluation of the semivariogram (univariate case) or cross-variogram (multivariate case). Because kriging uses an optimized search neighborhood for generating spatial estimates (the variogram is used to identify the distance over which properties are correlated), it is highly sensitive to the sample coverage, sample support, sample interval, and extent, which should be considered during the sampling design phases.

▼*Read more*

Kriging is known as the best linear unbiased estimator because:

- The search neighborhood weights are chosen so that the estimator is unbiased (difference between the predicted value and measured realization equals zero).
- Kriging solves a series of linear equations (kriging system) by minimizing the kriging variance.

Different kriging methods are unique in their assumptions, constraints, limitations, and purpose. Popular kriging methods include ordinary kriging, indicator kriging, simple kriging (see conditional simulation), factorial kriging, and universal kriging. When more than one variable contributes to the kriging estimate in each of these methods, it is termed "co-kriging."

Kriging can also be used to upscale (estimate over a given area or volume) or downscale (estimate at a specific location). Block kriging is a form of upscaling spatial information across a sampling domain. Point, or punctual, kriging is a means for downscaling spatial information across a sampling domain. The use of point or block kriging can be guided by the relationship of the sample design (support and spacing) to the interpolation grid cell size.

Often, many different types of data are collected from a contaminated site to directly and indirectly assess factors controlling the fate and distribution of contaminants. In soil systems, for example, it is common to integrate environmental geophysics, LiDAR, and soil sample information to characterize a site in space over time. Measured parameters that exhibit shared structured spatial variation (spatial autocorrelation or shared space-dependent variation) can be used together for interpolation, which is the process of co-kriging.

The search neighborhood is optimized through the cross variogram for co-kriging. Co-kriging is popular for integrating a high-resolution data set with a more sparsely sampled data set to generate spatial estimates with greater coverage. Co-kriging can be applied as block co-kriging or point co-kriging.

Data Transformations

▼*Read more*

Collected data often has a skewed distribution, which can introduce significant bias in the geospatial estimates, for example, when using ordinary kriging. In this case, the mean of the distribution is not representative of the data set. Ordinary kriging, also called the mean interpolator, performs the estimates of concentrations by using local means and the estimated values will be closely calculated around this mean. When an asymmetric distribution is observed, the kriged data histogram will not be consistent with the histogram of the original data.

Performing logarithmic or Gaussian (normalizing) transformations of the raw distributions may remediate this effect. If they are being used, data transformation should be completed before proceeding with kriging methods. Moreover, Gaussian (normal) distributions are needed to perform the conditional simulation method. This type of distribution may minimize the influence of high values compared to the low ones, and reveal the best data distribution in order to obtain a more structured experimental variogram

Below are general descriptions of point kriging and block kriging. These kriging approaches can be applied to all kriging methods discussed in this section.

Point and Block Kriging

▼*Read more*

Point kriging is one of the most common forms of kriging. Point kriging generates a point-estimated value of a sampled property at an unsampled location, using optimally weighted, known (sampled) ambient values. Point kriging is useful for estimating or simulating a measured property at finer spatial resolutions than was used in sampling (downscaling). Point

kriging estimates are sensitive to local discontinuities and large nugget effects.

Block kriging estimates a weighted average across a particular domain, in this case a grid cell or block. A predefined, regular-spaced interpolation grid is necessary to perform block kriging, which is ideal for studying regional patterns of variation, but not for local-scale variation. Block kriging inherently generates smoother maps than point kriging, helping to negate the effects of discontinuities in the data as well as other undesirable artifacts. The block kriging variance is lower in comparison to point kriging because the local scale variation, or within-block variation, is removed—an advantage for data sets with a large nugget.

Simple Kriging

Simple kriging assumes that the mean of the data is constant and known, which is a restrictive assumption. Consequently, ordinary kriging is preferred because it assumes that the mean is unknown and must be estimated from the data. Simple kriging is not recommended to be used by itself, but is regularly applied in conditional simulation.

Typical Applications

▼*Read more*

Simple kriging is used for spatial interpolation when the mean and spatial correlation model are constant and known. Simple kriging is applied in conditional simulation.

Using this Method

▼*Read more*

This method is subject to the following constraints:

- Data are second-order stationary if covariance function model is used or intrinsically stationary if variogram model is used.
- Spatial correlation is present among the data.
- No duplicate sites are present.

The spatial correlation model for kriging can be based on either the covariance function or variogram. In general, it is easier to estimate a variogram model than a covariance function because no estimate of the mean is required.

The pure nugget effect indicates the absence of spatial correlation. In this case, a deterministic geospatial method should be considered.

Assumptions

▼*Read more*

This method assumes the mean and variance are constant and known (second-order stationarity).

Strengths and Weaknesses

▼*Read more*

This method is very restrictive due to the requirement that the mean is known.

Understanding the results

▼*Read more*

In addition to interpolated values, kriging can provide an estimate of the uncertainty in the interpolated values, which is known as the kriging variance or standard error. The quality of the kriging model fit to the data should be evaluated using cross validation or validation.

In the context of optimization, see how to use the results of the geospatial methods to address specific optimization questions.

Ordinary Kriging

Ordinary kriging assumes that the overall mean is constant, though unknown, and the variance is finite (the variogram has a sill value). The goal is to produce a set of estimates for which the variance of the errors is minimized. To accomplish this goal, ordinary kriging weights each sample based on its relative distance from the location of the data point to be predicted.

Typical Applications

▼*Read more*

Ordinary kriging is used to generate estimates of a sampled variable in unsampled locations.

Using This Method

▼*Read more*

This method is subject to the following constraints:

- Intrinsic stationarity—the variogram has a sill.
- No duplicate sites are used.
- The nugget is small relative to the sill.

The spatial correlation model for kriging can be based on either the covariance function or variogram. In general, it is easier to estimate a variogram model than a covariance function because no estimate of the mean is required.

A pure nugget effect observed in the variogram indicates the absence of spatial correlation (strict stationarity). A variogram with a large nugget relative to the sill indicates variability in the data that cannot be accurately predicted using kriging. The nugget effect and shape of the variogram near the origin have the most influence on the kriging predictions. Since observations located beyond the range indicated by the variogram are spatially uncorrelated, the range can be used to select the kriging search radius.

Assumptions

▼*Read more*

- The data are locally stationary within the kriging search neighborhood.
- Data are locally second-order stationary if covariance function is used or intrinsically stationary if variogram is used.
- The data are spatially dependent.
- The expected value of a sample is the mean of the population.
- The difference in values between two samples is due to the distance between the two locations.

Strengths and Weaknesses

▼*Read more*

This kriging method is flexible enough to give good results for most data sets, unless there are strong spatial trends.

Understanding the results

▼*Read more*

In addition to interpolated values, kriging can provide an estimate of the uncertainty in the interpolated values, which is known as the kriging variance or standard error. The quality of the kriging model fit to the data should be evaluated using cross validation or validation.

In the context of optimization, see how to use the results of the geospatial methods to address specific optimization questions.

Further Information

▼*Read more*

Universal Kriging and Kriging with External Trend

Alternatives to ordinary kriging are universal kriging and kriging with external trend. Kriging with external trend is also known as kriging with external drift. These methods do not assume that the mean is constant, or even known, and assume that the trend that predicts the value of Z(s) can be modeled using a simple linear regression. If the linear regression for the trend uses only the spatial coordinates (for example, easting and northing) as explanatory variables, the method is called universal kriging. The form of regression commonly used with universal kriging is linear or quadratic, but any form can be used. Both the regression coefficients and kriging weights are estimated simultaneously by universal kriging.

If the regression uses other quantities as explanatory variables, the method is called kriging with an external trend. For

example, the drawdown around a pumping well can be predicted using the Theim equation, which is a function of the distance from the pumping well. The trend in groundwater levels near the well can be included in the kriging method using a regression form of the Theim equation, with distance to the well as the explanatory variable. Kriging with an external trend fits the measured water levels at monitoring wells by adjusting both the regression coefficients and the kriging weights.

Typical Applications

▼*Read more*

Universal kriging and kriging with an external trend are used for spatial interpolation when there is a trend in the data. In applications for remediation optimization, this approach may include distribution of contaminant concentrations from a single point source.

Using this Method

▼*Read more*

It is necessary to develop a model of the semivariogram or the covariance function. Several software packages can be used to perform the necessary operations, with varying requirements for user expertise.

Assumptions

▼*Read more*

- Data have a spatial trend that is modeled using a simple function of the location coordinates.
- Detrended data are locally second-order stationary if covariance function is used or intrinsically stationary if variogram is used.

Strengths and Weaknesses

▼*Read more*

Universal kriging provides the ability to interpolate spatially related values when there is a trend in the mean, a property not realized with ordinary kriging. However, the use of universal kriging is limited to scenarios in which the variation exhibited by the attribute of interest can be considered to be systematic. As with most interpolation techniques, the uncertainty associated with the results of the method increases dramatically with the complexity of the model used, and should be taken into account.

Understanding the Results

▼*Read more*

In addition to interpolated values, kriging can provide an estimate of the uncertainty in the interpolated values known as the kriging variance or standard error. The quality of the kriging model fit to the data should be evaluated using cross validation or validation.

In the context of optimization, see how to use the results of the geospatial methods to address specific optimization questions.

Further Information

▼*Read more*

Indicator Kriging

Indicator kriging method is a nonparametric variant of ordinary kriging using data indicator variables that are defined using binary values (0 or 1) based on whether the data exceed a specified threshold (such as the remediation goal). The value assigned to the sample points exceeding the specified threshold is 1. The assigned value is 0 for the sample points below this threshold.

Typical Applications

▼*Read more*

This method is typically used to map the probabilities of exceeding the specified threshold.

Using this Method

▼*Read more*

The concentrations must be transformed into a binary variable (0,1). Several variograms must be developed and fitted if several thresholds are set.

The verifications that must be performed in order to implement this method are:

- the coherence between the variograms constructed for each indicator
- the cross validation for each variogram model and the neighborhood (taken into account for the interpolation)
- the variance map

Assumptions

▼*Read more*

This method assumes stationarity of each indicator.

Strengths and Weaknesses

▼*Read more*

The advantages of indicator kriging method include:

- The method does not require any assumption about data distribution.
- The method can be used for categorical data (type of soil, index of contamination).

The weaknesses of this method are:

- The same value (1) is assigned for all the sample points exceeding the specified threshold. The degree of contamination is not taken into account. This means a result several orders of magnitude above the threshold has the same effect on nearby exceedance probability as a result that is less than 1 percent above the threshold.
- A variogram must be constructed and fitted for each indicator corresponding to each threshold.
- The use of a nugget effect is questionable for an application where it is assumed that comparisons to a threshold value are exact (Krivoruchko and Bivand 2009).
- Negative probabilities or probabilities greater than 1 may appear because of the weights applied by the kriging or if the variograms for each threshold are not compatible.

A major limitation to kriging techniques and their associated estimates of exceedance probability is that these methods minimize the variance to generate spatial estimates. This result inherently underestimates the variability of the system being characterized and thereby biases the probability outcomes. An alternative to kriging that overcomes this limitation is conditional simulation.

Understanding the results

▼*Read more*

The results obtained by performing indicator kriging are expressed in terms of probability. Thus, mapping of the results does not indicate the concentrations of the contaminants, but rather the risk of exceeding a threshold such as the remediation goal.

In the context of optimization, see how to use the results of the geospatial methods to address specific optimization questions.

Other Kriging Methods

Probability Kriging.▼*Read more*

Probability kriging and disjunctive kriging are two alternatives that can overcome some of the limitations of indicator kriging. Probability kriging uses autocorrelation of both the original data and the indicator binary variable, and cross-correlation between them. Probability kriging uses co-kriging to preserve some of the information lost in indicator kriging (ESRI 2013).

Disjunctive Kriging▼*Read more*

Disjunctive kriging is defined as the simple kriging of data transformed to a standard normal distribution using Hermite polynomials. A probability distribution and associated map of probabilities can then be generated by comparing estimated

values with the normal distribution (Webster and Oliver 2001). Disjunctive kriging assumes that the data in question follow a bivariate normal distribution. This assumption means that linear combinations of paired values are normally distributed with correlation coefficients depending solely on separation distance rather than absolute position (Krivoruchko 2011). Probability kriging is available in ArcGIS Geostatistical Analyst, and disjunctive kriging is available in ArcGIS Geostatistical Analyst, Isatis, and R.

Regression Kriging. ▼*Read more*

Regression kriging is a hybrid of regression and kriging methods. A regression to predict the quantity of interest based on auxiliary variables (such as land surface elevation or soil type) is performed first, and then simple kriging is performed on the regression residuals. This method is mathematically equivalent to kriging with external drift (trend), where the auxiliary variable relationship and kriging model is solved simultaneously to calculate the kriging weights. The advantage of regression kriging is that it can extend the method to a broader range of regression techniques and allow separate interpretation of the two interpolated components.

Factorial Kriging Analysis (FKA) ▼*Read more*

Factorial Kriging Analysis (FKA) involves multivariate variogram modeling, principal component analysis, and co-kriging. Factorial kriging allows investigators to simultaneously study spatial relationships between multiple variables according to their shared spatial ranges of autocorrelation. Three primary outputs are generated from this technique:

- regionalized correlation coefficients
- regionalized factors (principal components)
- individual sets of concentration maps (univariate) and principal component maps (multivariate)

Spatial autocorrelation implies that a fraction of the total measured variation in the data are space dependent, or structured. Although several analytical tools can model spatial autocorrelation, the variogram is the fundamental component of factorial kriging.

Co-kriging

In general, co-kriging is used only when the primary variable is under-sampled and the secondary data are spatially correlated with the primary variable (Goovaerts 1997). Direct measurements, such as those obtained from soil cores and geologic borings, are also referred to as primary sampling and are often limited in spatial coverage because of their cost, accessibility requirements, manpower, or invasiveness. Sparse direct measurements can prove inadequate for capturing the underlying spatial or temporal autocorrelation of a property or process of interest. When primary sampling is limited, it can be advantageous to incorporate secondary sampling technologies as supplementary site characterization tools. An example application of co-kriging is included.

▼*Read more*

Integrating densely sampled secondary measurements can lead to more consistent descriptions of sparsely sampled direct measurements (Castrignanò et al. 2012). When the secondary variable is sampled much more densely than the primary variable, however, it can cause instability in solving the kriging system because the correlation between close secondary data is greater than that of sparse primary data (Goovaerts 1997). Collocated co-kriging is an efficient method to integrate exhaustive secondary measurements with sparse primary measurements to estimate the primary variable at target locations (Morari, Castrignanó, and Pagliarin 2009). Collocated co-kriging is similar to ordinary co-kriging, except that the neighborhood search specifically uses the secondary variable information collocated with the measured primary variable and the target location to be estimated. In depth discussion of collocated co-kriging is beyond the scope of this document; suggested readings on this topic include Goovaerts 1997; Castrignanò et al. 2012; and Morari, Castrignanó, and Pagliarin 2009.

Conditional Simulation

Conditional simulation is the most robust way to create exceedance probability maps. A major limitation to kriging techniques is that the methods minimize the variance to generate the spatial estimates. This result inherently underestimates the variability of the system being characterized and biases the probability outcomes. Conditional simulation is a nonlinear method designed to produce fields showing the same spatial structure (variogram) and the same histogram as the original data. The simulations must ensure that each field is consistent with the observed values on the sample points if the nugget value is zero. Thus, if a value is simulated at a point coinciding with an observation, the simulated value must be equal to the observed value.

Sequential Gaussian simulation is the most commonly used method to develop conditional simulations and is included in several software packages.

Sequential Gaussian Simulation

This method generates each x value one-by-one by using kriging. Values are based on the kriging mean and variance obtained at the location x_i from the data. The term Gaussian is derived from the use of normal (Gaussian) conditional distributions, functions, and parameters.

The basic approach of sequential Gaussian simulation is to generate a random path for each point to simulate. This method generates a conditional distribution which is also a Gaussian (normal) distribution, whose expectations and variances can be deduced from simple kriging. The sequential Gaussian simulation method transforms the bivariate distribution into a univariate distribution. The size of the kriging increases with each additional simulated point. Kriging can be limited to a moving neighborhood; however, errors (artifacts) may occur if the neighborhood is too small.

Typical Applications

▼*Read more*

The results obtained by performing conditional simulation have several applications:

- mapping the contamination sources according to a remediation goal
- mapping the uncertainties associated with the estimates in order to determine the financial risk of the project
- defining new sampling programs according to the mapped uncertainties
- defining the strategy for cleanup

Using this Method

▼*Read more*

This method requires a Gaussian transformation of the original data set. Several techniques allow the transformation of the raw data to a Gaussian distribution (for example, Hermite polynomials, Gaussian anamorphosis). In order to produce a conditional simulation, a new variogram must be developed with the Gaussian distribution and then fitted. Variogram development and simulations must be performed on Gaussian transformed data and results must be back-transformed.

Assumptions

▼*Read more*

This method assumes normal distribution and second order stationarity if simple kriging is used.

Strengths and Weaknesses

▼*Read more*

The advantages of the conditional simulation method are:

- Each simulation respects the values observed in the sample points. Mean and variance are preserved in each realization.
- Performing a large number of simulations better reproduces the real diversity of possible cases, when random variables are modeled.
- It is possible to quantify and locate the areas of uncertainty and to support management of the financial risks of a project.

The weaknesses are:

- Some distributions do not allow a perfect Gaussian transformation of the data set.
- The time for completion can be longer than other methods.
- Because of the large data sets generated, computation time may be significant.

Understanding the Results

▼*Read more*

The results of conditional simulation are expressed by a number of equally probable maps. Each realization obtained by using the conditional simulation method is equally valid (Figure 81).

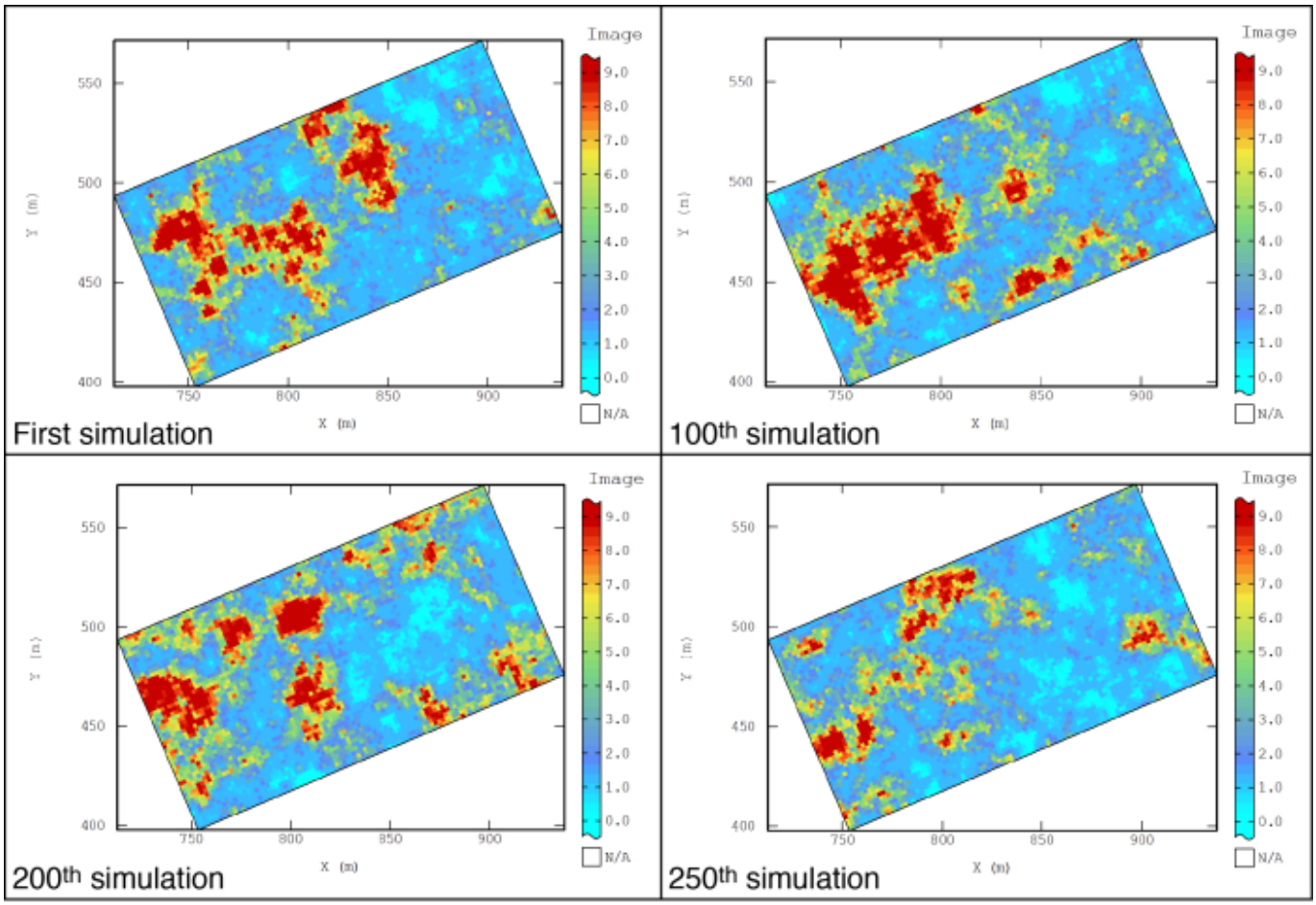


Figure 81. Conditional simulation results.

Which is the most appropriate model to represent the contamination? A simulation postprocessing step compiles the set of models produced by this method. The objective of this postprocessing is to answer the following questions:

1. *A) What are the contaminated areas?* This question is used to locally estimate the risk of exceeding a remediation threshold.

When a remediation threshold is applied, a first postprocessing can be performed in order to estimate the local level of contamination within each block. For example, a block x is simulated a hundred times. If this block x exceeds the remediation threshold 20 times, then the local probability of exceeding the threshold for this block x is 20%. This process is repeated for each block of the grid.

The final maps are expressed in terms of probability which defines the contamination risk within each block according to the remediation threshold. Figure 82 shows the results.

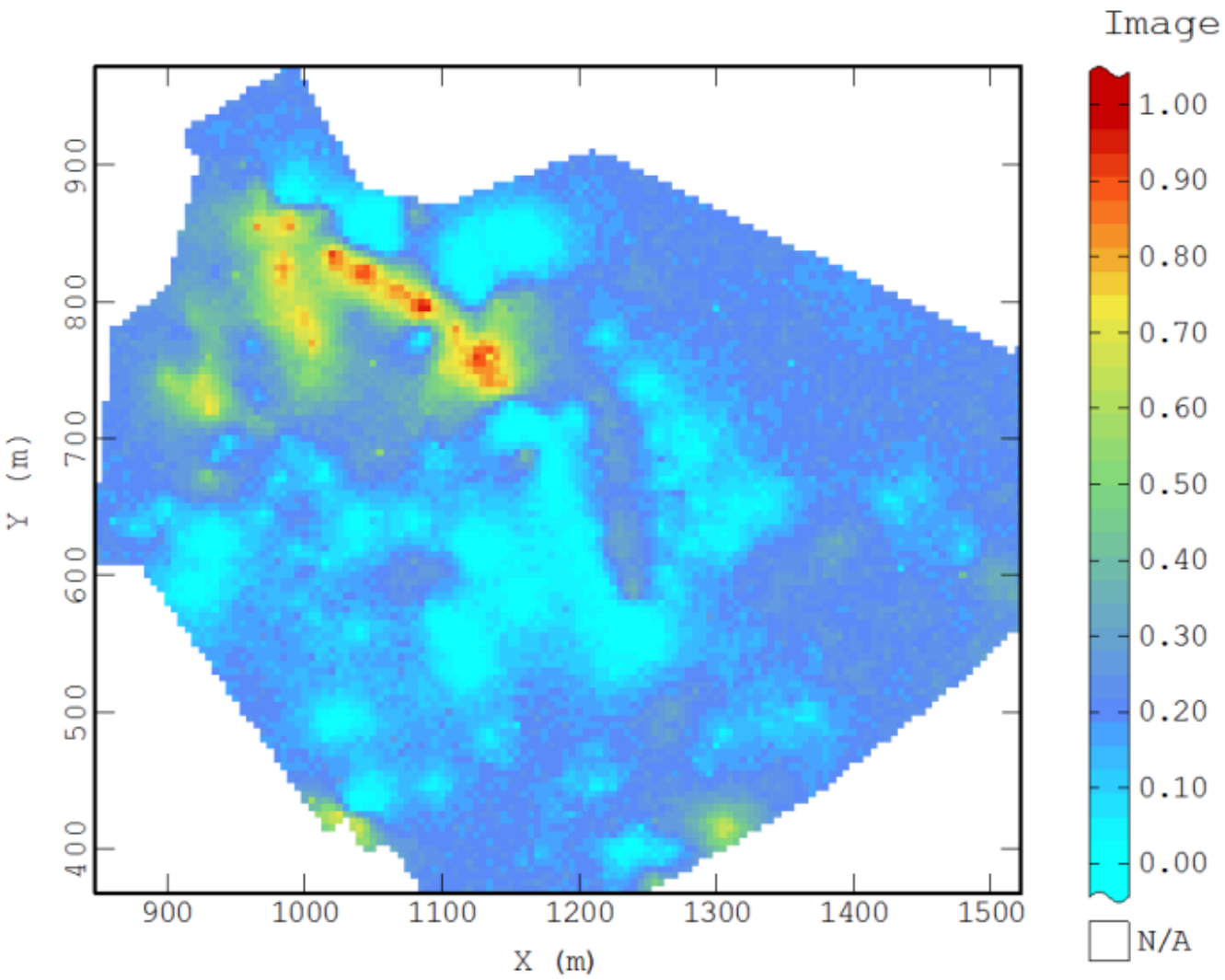


Figure 82. Probability map.

1. *B) What is the contaminated volume?* This question is used to estimate the overall level of contamination in the study area.

Similarly, the postprocessing of conditional simulation allows you to estimate the overall degree of contamination on the site. If a hundred simulations are performed, the contaminated volume can be calculated for each realization, by calculating the number of blocks showing concentrations above the remediation threshold. Thus, if a hundred simulations are performed, a hundred volumes of contamination will be obtained. This technique allows you to define the overall degree of contamination on the site and to define a margin of error by obtaining the optimistic and pessimistic volume (percentiles 5 and 95) and the most probable volume (median of the distribution). Figure 83 shows the results of this technique.

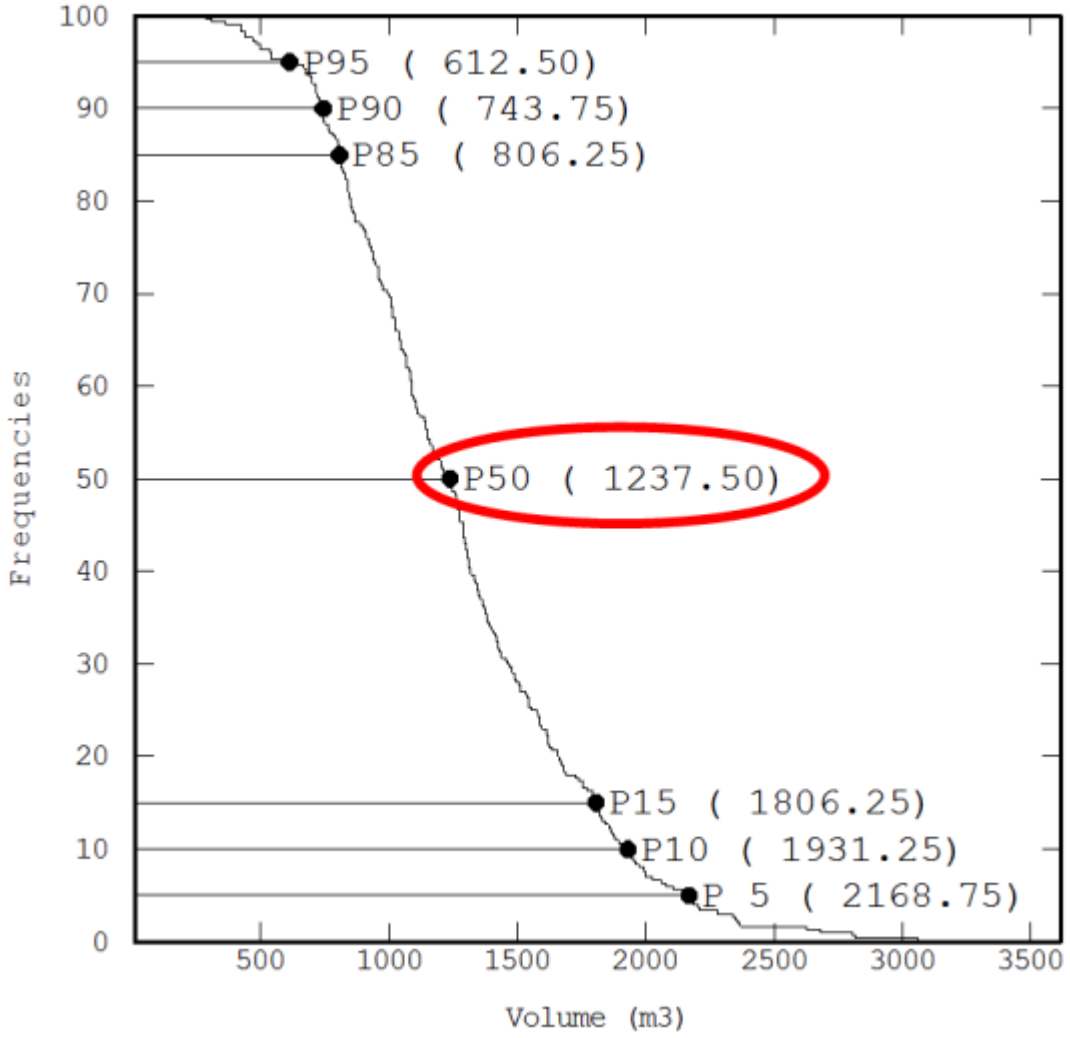


Figure 83. Using conditional simulation results to determine probable volume of contamination.

An accurate estimate minimizes the differences between the optimistic and the pessimistic volumes.

Furthermore, other maps can be produced to better interpret the results:

- mean of the realizations: a map similar to the results obtained by kriging
- smallest and largest realizations: shows the optimistic and the pessimistic mappings obtained by performing the conditional simulation
- standard deviation of realizations: quantifies the error of the estimation within each block and gives an estimate of the calculation accuracy

The verifications that must be performed in order to implement this method are:

- Gaussian transformation of the data set
- cross-validation for the variogram model and the neighborhood taken into account for the interpolation
- quantification of the uncertainties and the differences between the optimistic and pessimistic volumes in order to determine the measure of certainty of the estimates.

In the context of optimization, see how to use the results of the geospatial methods to address specific optimization questions.

Co-Simulation

Co-simulation is an advanced method that is used for estimating values for a primary variable when there are secondary data available (known as proxy data). It is similar to conditional simulation. In co-simulation multiple values are generated for the primary variable at unsampled locations using both the primary and secondary sampled data. The values are generated using a probability simulation technique. Like co-kriging, co-simulation is used when the primary variable is under-sampled and the secondary data are spatially correlated with the primary variable. A cross variogram is used to check the spatial correlation; see co-simulation for estimating concentrations based on proxy data.

Further Information

▼*Read more*

- "PAH contamination in sediments: Uncertainty analysis," case study that uses conditional simulation (Section 6.2)
- "The turning bands method for simulation of random fields using line generation by a spectral method" (Mantoglou and Wilson 1982)
- *Geostatistics: Modeling Spatial Uncertainty, Second Edition* (Chilès and Delfiner 2012)
- *Geostatistical Simulation, Models and Algorithms* (Lantuéjoul 2002)
- *Plurigaussian Simulations in Geosciences* (Armstrong et al. 2011)
- *Introduction to Disjunctive Kriging and Nonlinear Geostatistics* (Rivoirard 1994)