Geostatistics - Uncertainty quantification: examples

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Summary

The multiGaussian and the indicator approaches are used to determine local point uncertainty over one of the domains of the deposit used previously to illustrate the concepts. We show the implementation steps and discuss the differences in the results. We discuss the importance of tail extrapolation in the indicator framework.

Particular attention is given to the difference in uncertainty in the models by looking at the conditional variances, and their relationships with the estimates.

1 Example

1.1 MultiGaussian kriging

Steps

To implement multiGaussian kriging, we need:

- **Representative distribution**: the raw data distribution needs to be declustered.
- **Normal scores transformation**: the original raw data must be converted into a standard Gaussian distribution through a quantile transformation. The quantiles are assessed over the representative (declustered) distribution.
- **Variogram of normal scores**: since the estimation is done over the normally transformed data, the spatial continuity is required for the transformed data. An experimental variogram of the normal scores is inferred and modeled. The main features of the spatial continuity should be the same as those of the original variable (before transformation). Therefore, the same anisotropy directions can be used. However, the variogram of normal scores will be smoother and better behaved than the one of the raw variable, since the effect of outliers will be considerably reduced, giving more reliable experimental variogram values. The anisotropy ratios tend to be reduced, that is, the normal scores variogram looks more isotropic than that of the original variable.
- **Point kriging of the normal scores**: in theory, the simple kriging estimate and variance of normal scores correspond to the conditional expectation and conditional variance at the unsampled location, under the multiGaussian assumption. Only point support estimation can be used, since the transformation from the

original data to the normally transformed values is a non-linear function, thus an average in normally transformed units will not match the corresponding average in original units, after back-transformation.

- **Back-transformation**: the conditional distribution of the normally transformed values is a Gaussian distribution centered at the simple kriging estimate and with a spread corresponding to the simple kriging variance. A quantile back-transformation can be done to recover the conditional distribution in original units.
- **Post-processing**: the conditional distributions in original units can be post-processed to obtain an estimate (in original units), its conditional variance and any other statistics, since we have the full local histogram.

Normal score transformation of declustered histogram

The declustered histogram of copper grades is used to build the transformation table where the quantiles are matched to those of a standard Gaussian distribution.

The samples are then transformed and a normal score is assigned to each sample. Notice that these samples are still clustered in space, so if we were to build the histogram of normal scores, it would be over representing some areas with more samples (likely higher grade areas that translate into higher normal scores). Declustering weights should be used to build the representative histogram of the normal scores, which by design is a standard normal histogram.

Figure 1 shows the declustered grade histogram and the corresponding declustered normal scores histogram. It can be seen that the former follows a perfect normal distribution with mean 0 and variance 1, when accounting for the declustering weights.

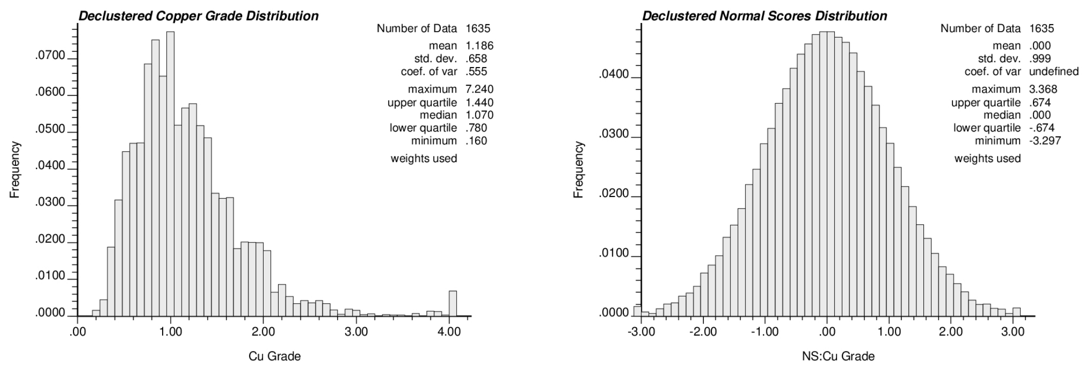

Figure 1: Declustered grade histogram and declustered normal scores histogram.

Variogram of normal scores

The parameters used previously to compute the experimental variogram of the grades are used now for the normal scores. The result in the main directions of anisotropy is quite smooth and easier to model than in the case of the original variable.

Figure 2 shows the model for the variogram of normal scores and the fit over the experimental curves in the principal directions. **Table 1** shows the parameters for the variogram model of the normal scores.

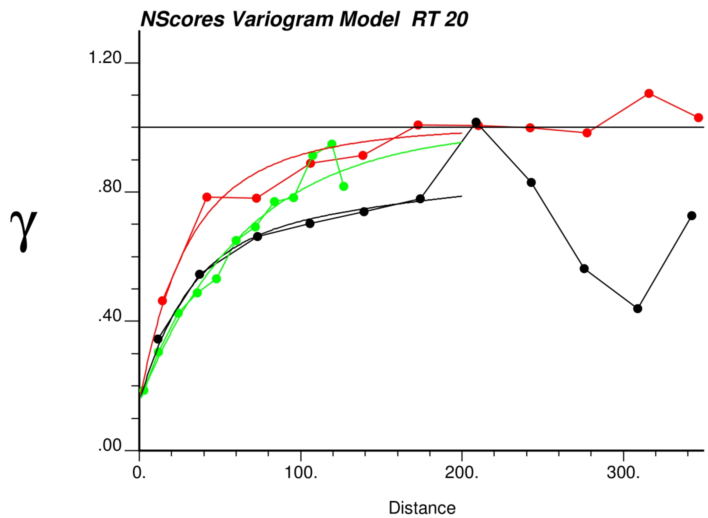

Figure 2: Experimental variogram of normal scores and model in three principal directions.

Type	Sill	Angle 1	Angle 2	Angle 3	Range Y”	Range X”	Range Z”
Nugget	0.15						
Exponential	0.50	30	0	0	70	90	180
Exponential	0.35	30	0	0	200	1200	240

Table 1: Parameters of the variogram model of normal scores

Simple kriging of normal scores

Simple kriging is applied over a point-support grid, because change of support cannot be done over the transformed variable. The transformation is non-linear (**Figure 3**), therefore, an average on Gaussian transformed values will not match the corresponding average of their back-transformed grades.

In this case, multiGaussian kriging is executed using a minimum of 8 and maximum of 16 samples within a neighborhood with a radius of 100 m. Notice that because of the need to make a global transformation of the histogram, a stronger assumption of stationarity is implicit. The conditional expectation and variance will be obtained exactly by simple kriging of the normal scores, as long as their distribution is multiGaussian and stationarity holds.

The result (before back-transformation) is presented in **Figure 4** for the estimates and for the estimation variance. It can be seen that the values range from approximately -3 to +3, and that the variance reflects the amount of information available. The sample locations appear clearly in the map of estimation variances. Also, we can see that the variances range from 0 to 1, since the prior variance of the normal scores is 1.

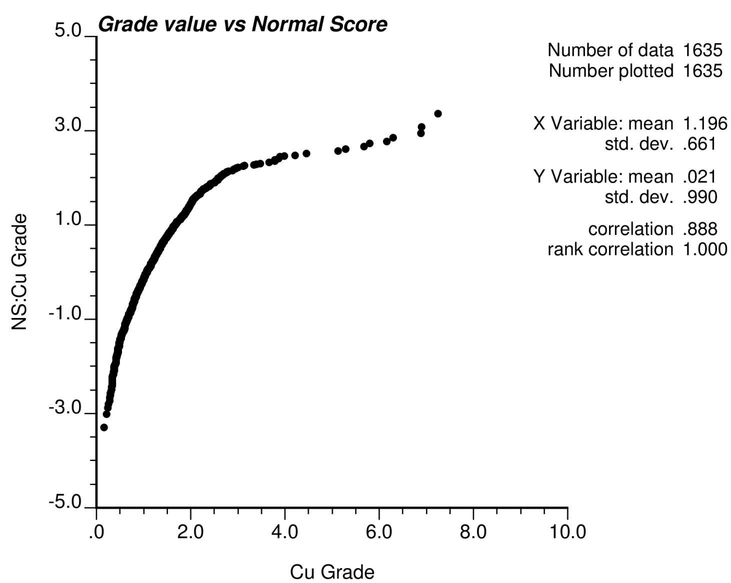

Figure 3: Non-linear relationship between grades and normal score transforms.

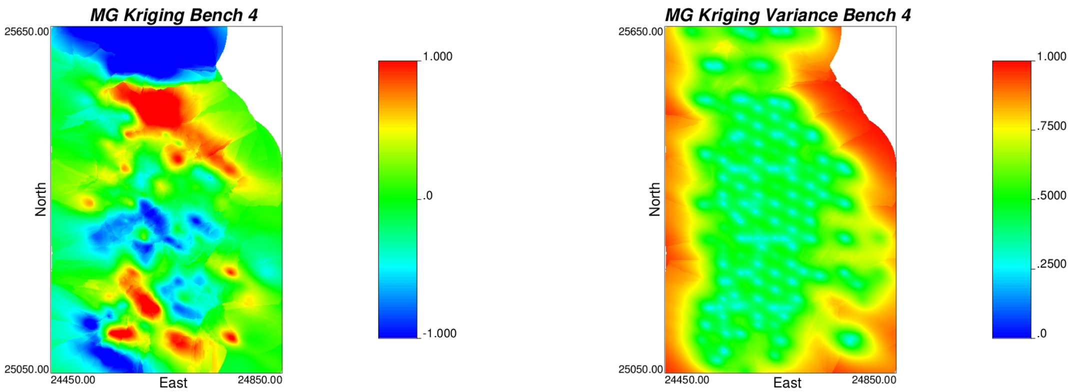

Figure 4: Normal score estimates and variance by simple kriging.

Back-transformed estimates and variances

At every point in the estimation grid, a mean and variance of the conditional distribution in Gaussian units is available. Under the multiGaussian assumption, the conditional distribution is Gaussian in shape, thus by knowing the mean and the variance we know it completely. We can back-transform as many quantiles as required to obtain the back-transformed conditional distribution (now in grade units).

Resulting maps depicting the estimated value (mean) and conditional variance are shown at the top in **Figure 5**. For comparison, the ordinary kriging estimate and variance maps at point support obtained previously are displayed at the bottom of the same figure. It can be seen that the estimates follow similar trends and are not significantly different, except in areas where extrapolation occurs. MultiGaussian kriging is based on simple kriging, thus tends to bring extrapolated values back to the mean, while the ordinary kriging estimates rely on the average obtained in the local neighborhood. More interesting is the behavior of the variances. In multiGaussian kriging, the variance (after back-transformation) is proportional to the estimate.

Histograms of estimates and variances are presented prior to back-transformation and after back-transformation in **Figure 6**. Notice that the estimated values in Gaussian units are smoother than the prior (global) distribution, which had a variance of 1. Also, it is apparent that the distribution of estimates is not exactly Gaussian in shape. Estimation variances in Gaussian units are bimodal. This is probably due to the data configuration. Regarding the back-transformed estimates and variances, it can be seen that the estimate is smoother than the original grade distribution and more symmetric. The kriging variance histogram shows a long tail of high variance values.

Estimates and variances in grade units obtained with multiGaussian kriging and with ordinary kriging are compared in the scatter plots provided in **Figure 7**. A slight global bias is apparent between the estimates, which is probably due to the areas where the grades are extrapolated. When looking at the global statistics, these are summarized in **Table 2**, we can see that ordinary kriging averages approximately 2% lower than the statistics obtained by cell declustering (which are not very reliable in the first place). MultiGaussian kriging assumes global stationarity on the mean, thus if significant extrapolation areas exist, it may generate incorrect results. Nonetheless, the bias is not significant.

On the other hand, we can see in **Figure 7** that the ordinary kriging variance and multiGaussian kriging conditional variance are not correlated in a simple manner. The global correlation coefficient is close to zero, indicating that these

Method	Mean	Std. Dev.	Bias
Declustered distribution	1.186	0.658	–
Ordinary kriging	1.163	0.476	-1.9%
MGK (simple kriging)	1.146	0.385	-3.4%

Table 2: Mean and standard deviation of declustered distribution and estimated points with ordinary kriging and multiGaussian kriging in unit 20.

two measures of “uncertainty”, are completely different. As seen in **Figure 4**, the conditional variance is proportional to the estimated value, while the ordinary kriging variance is not dependent on the estimated values and only reflects the amount of information in the neighborhood.

Comments

The proportional effect can be understood by looking at the scatter plots between estimated values and estimation variance. **Figure 8** shows the scatter plots before and after back-transformation. Before back-transformation the estimate and variance are unrelated, while after back-transformation, the estimated grade is clearly related to the conditional variance in grades units. In fact, since the distribution is close to a lognormal, this relationship is quadratic (and linear between the estimate and the kriging standard deviation).

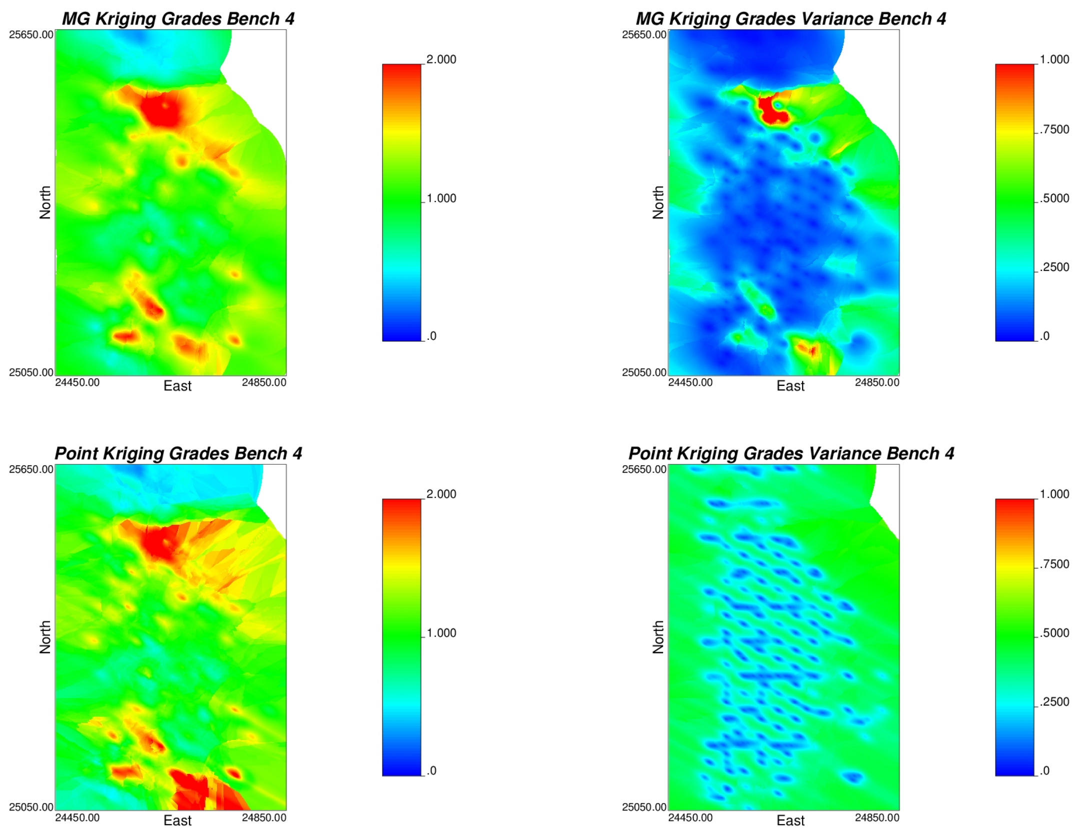

Figure 5: Maps of estimates and estimation variances for multiGaussian kriging and for ordinary kriging (obtained previously).

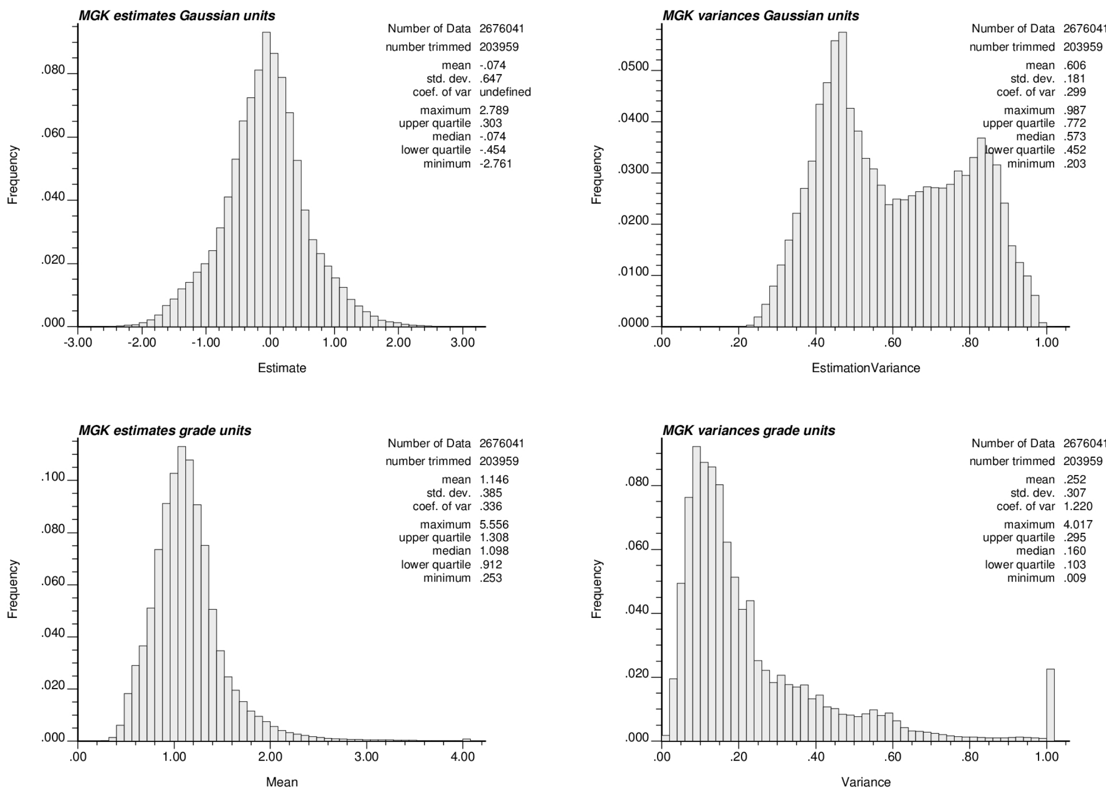

Figure 6: Histograms of estimates and estimation variances for multiGaussian kriging values in Gaussian units (before back-transformation), at the top, and in grade units (after back-transformation), at the bottom.

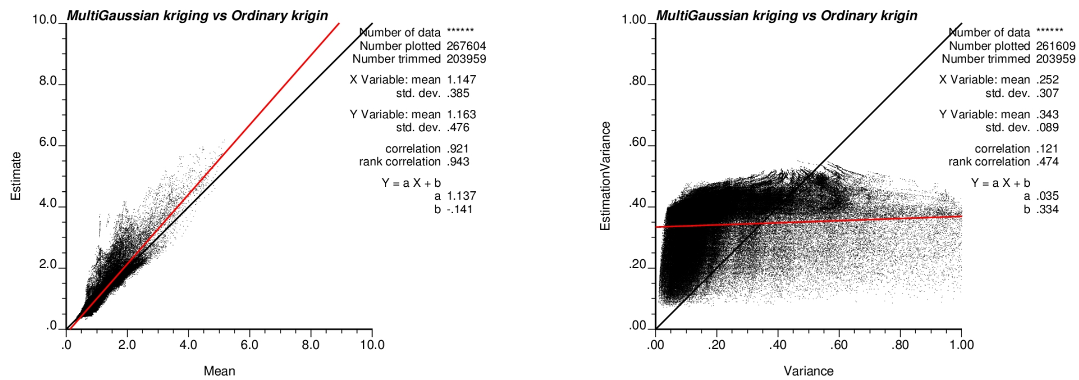

Figure 7: Comparison of estimates and estimation variances for multiGaussian kriging and for ordinary kriging (obtained previously).

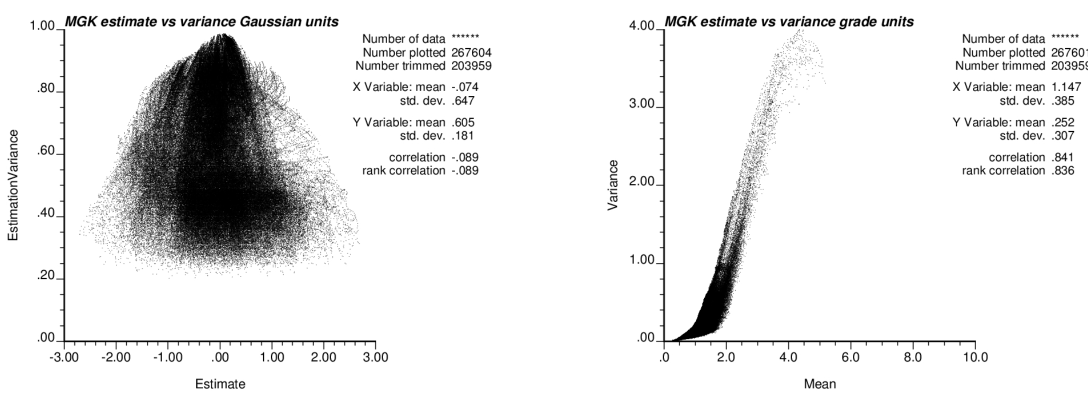

Figure 8: Proportional effect. Left: the relationship between estimate and variance in Gaussian units, showing no relationship. Right: the relationship between estimate and variance in grade units, after back-transformation, showing the proportional effect.

1.2 Multiple indicator kriging

Steps

To implement multiple indicator kriging, we need:

- **Representative distribution**: a declustered distribution is needed prior to the definition of the thresholds used to define the indicators.
- **Definition of thresholds**: the number of thresholds and their values need to be determined. They are usually defined to evenly sample the global distribution, and a few thresholds are added to account for relevant values (cutoffs in mineral resource estimation, or critical thresholds in pollution studies) and to characterize the tail of the distribution. Thresholds can be defined at regular quantiles (for example over the deciles of the distribution) and some additional thresholds may help discretizing the tail. Notice that as thresholds get extreme (lower or higher), their spatial structure tends to be difficult to discern during the variogram analysis, so unless a good amount of sample data is available, it is not advisable to select thresholds too extreme.
- **Indicator variogram analysis**: a kriging run is performed for each indicator, therefore, the spatial continuity of each indicator is needed. Variogram models must be created for all the indicator variables. Good practice is to have all variogram models with the same base structures and change the sills and ranges smoothly from one threhold to the next avoiding abrupt changes.
- **Point support indicator kriging**: kriging is performed independently for each threshold. Simple or ordinary

kriging can be used. Estimation must be done at point support.

- **Post-processing of the conditional distributions**: the resulting indicator estimates discretize the conditional distribution at every location. These points must be interpolated and extrapolated to complete the conditional distribution. This may require correcting for order relation problems. Once this has been done, the full conditional distribution can be used to obtain the local mean, variance and any other statistics required, by numerical integration.

Determining the thresholds

The thresholds for the case study are defined at regular intervals in probability (deciles) and three additional thresholds are considered to characterize the tail of high values. These are summarized in **Table 3**.

Number	Cumulated Probability	Threshold
1	0.10	0.55
2	0.20	0.72
3	0.30	0.83
4	0.40	0.95
5	0.50	1.07
6	0.60	1.21
7	0.70	1.36
8	0.80	1.55
9	0.90	1.898
10	0.95	2.18
11	0.98	2.681
12	0.99	3.682

Table 3: Definition of thresholds for multiple indicator kriging in unit 20.

Indicator variograms calculation and modeling

Indicator variograms are computed in the three principal directions of anisotropy defined previously. For every threshold, the grades are transformed to a binary indicator and the corresponding variogram is computed. Notice that the experimental variograms are standardized to a sill of 1, which makes the modeling stage easier. Recall that the variance of the indicator variable is known and this should correspond to the sill of the indicator variogram (under the assumption of stationarity).

The models are summarized in **Table 4**. The experimental variograms and the fitted models are shown in **Figure 9**.

Number	Cumul. Prob.	Threshold	Nugget Effect	Exponential			Exponential		
				Sill	Angles	Ranges	Sill	Angles	Ranges
1	0.10	0.55	0.15	0.35	30/0/0	20/30/20	0.50	30/0/0	700/1300/180
2	0.20	0.72	0.15	0.45	30/0/0	20/30/15	0.40	30/0/0	280/520/180
3	0.30	0.83	0.15	0.35	30/0/0	40/45/15	0.50	30/0/0	120/220/180
4	0.40	0.95	0.18	0.32	30/0/0	50/60/15	0.50	30/0/0	100/180/180
5	0.50	1.07	0.18	0.32	30/0/0	50/80/25	0.50	30/0/0	100/160/180
6	0.60	1.21	0.15	0.35	30/0/0	70/70/15	0.50	30/0/0	100/140/200
7	0.70	1.36	0.15	0.35	30/0/0	70/70/15	0.50	30/0/0	100/140/200
8	0.80	1.55	0.15	0.35	30/0/0	55/70/45	0.50	30/0/0	85/140/160
9	0.90	1.898	0.15	0.35	30/0/0	10/20/45	0.50	30/0/0	50/110/160
10	0.95	2.18	0.15	0.35	30/0/0	10/10/35	0.50	30/0/0	40/80/200
11	0.98	2.681	0.15	0.35	30/0/0	10/10/45	0.50	30/0/0	40/80/200
12	0.99	3.682	0.15	0.35	30/0/0	10/10/55	0.50	30/0/0	40/80/200

Table 4: Indicator variogram model parameters

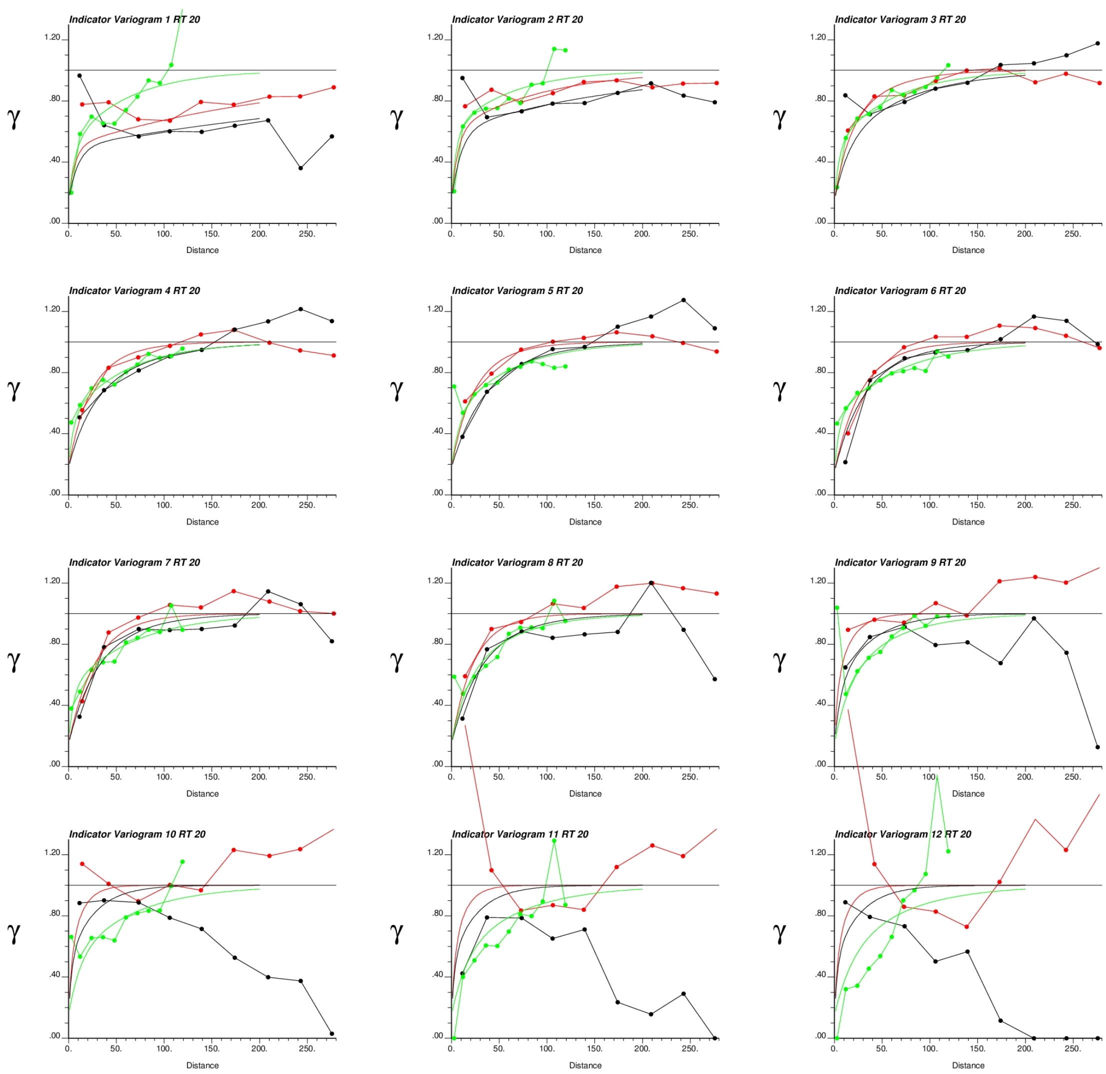

Figure 9: Experimental indicator variograms and models for unit 20.

It can be seen from the variograms, that high thresholds tend to generate very unreliable variograms. The models fit for the last few thresholds are really based on the model for lower thresholds. The fitting is poor, since the experimental variograms do not behave as expected. More effort could be put to improve the experimental variograms and the fit of the models.

Multiple indicator kriging

Multiple indicator kriging is essentially *K* independent runs of kriging, each with different data (the coding changes for each threshold) and different variogram (the model changes, as presented before). Typically, search parameters are kept constant for all thresholds. MIK is run over the same point support grid used previously for ordinary and multiGaussian kriging. A minimum and maximum of 8 and 16 samples are used, considering a isotropic search with radius of 100m. Ordinary kriging is used for each indicator and the median shortcut is not used, so each threshold uses its corresponding variogram model.

The output of multiple indicator kriging is a set of *K* models that predict the probability of not exceeding each one of the thresholds. The maps range from 0 to 1, as they represent probabilities. These are presented in **Figure 10**. There are some obvious artifacts due to the search parameters and extrapolation at the margins of the field.

Post-processing to obtain the estimate and conditional variance

The resulting probabilities at different thresholds provide an approximation of the local conditional distributions at every location of the grid. Parameters for “filling the blanks” are required, to complete the conditional distributions. Further-

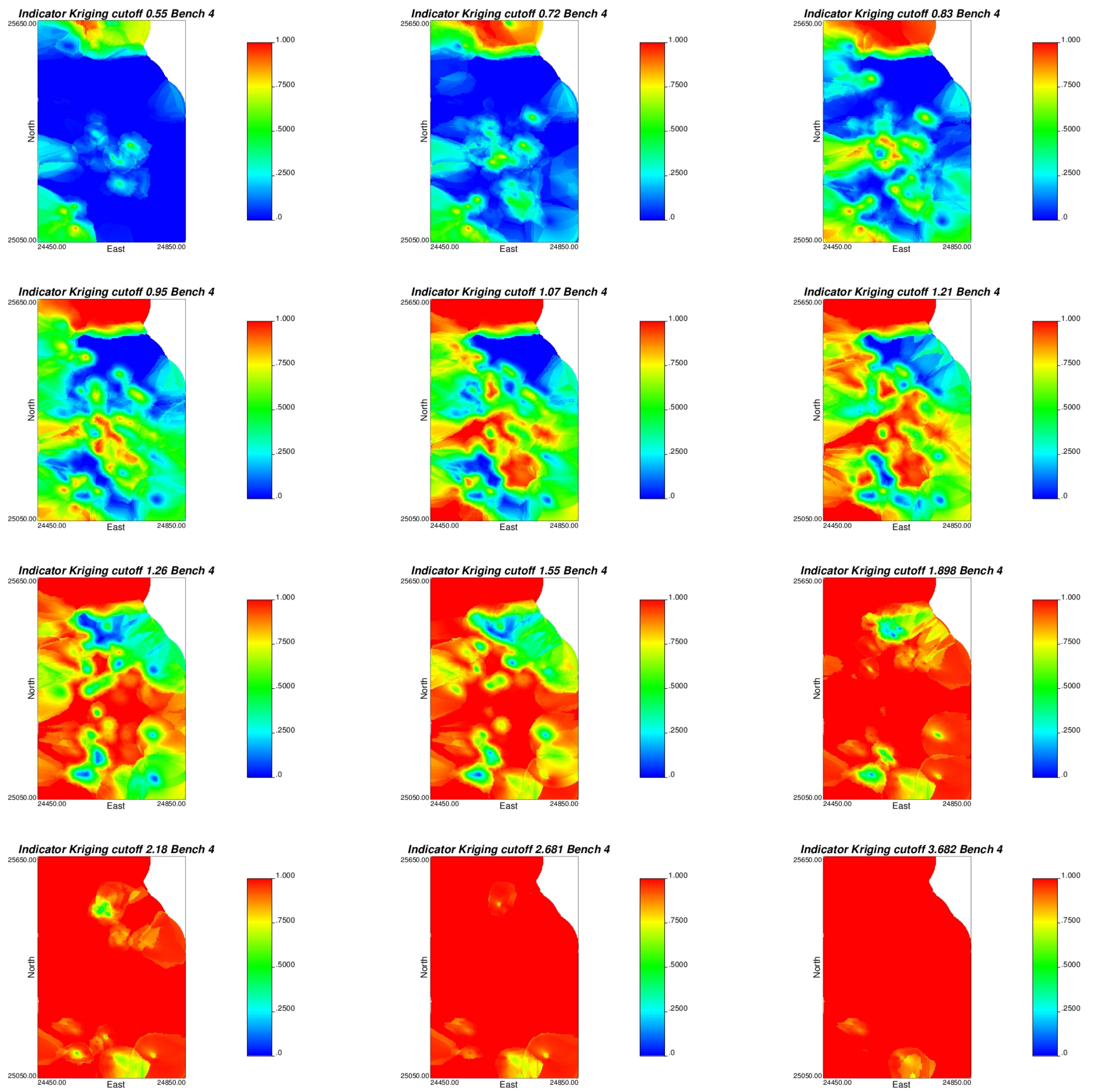

Figure 10: Maps for a representative planview of indicator kriging for each of the twelve thresholds (unit 20).

more, order relation problems need to be fixed, in case they exist. These problems arise from the fact that each kriging is run independently, when in reality, adjacent thresholds should be closely correlated.

Parameters for conditional distribution interpolation between thresholds and extrapolation beyond the first and last thresholds to a set minimum and maximum values, are presented in **Table 5**.

Case	Model	Parameter
Interpolation	Linear	—
Extrapolation lower tail	Linear	0.0
Extrapolation higher tail	Linear	7.5

Table 5: Parameters for conditional distribution interpolation and extrapolation.

With these parameters, the conditional distributions at every point in the estimation grid can be numerically integrated to obtain the mean and the conditional variance. Other statistics can also be obtained similarly, such as confidence intervals, median, quartiles, etc. The numerical integration is performed considering a discretization of 200 quantiles, both for the mean and variance. The resulting maps, after post-processing the indicator kriging output, are presented in **Figure 11** and compared to the corresponding ordinary kriging results.

In many cases, the model used for extrapolation of the higher tail may bias the result. Too heavy a tail may create an overestimation of the global mean. It is important to check the statistics and calibrate the result, if needed, to match the known declustered mean. Notice that this requires re-running the post-processing, but not necessarily modifying the indicator kriging run. Statistics for the estimate and variance are summarized in the histograms displayed in **Figure 12**. For comparison, **Table 2** is updated and provided below (**Table 6**).

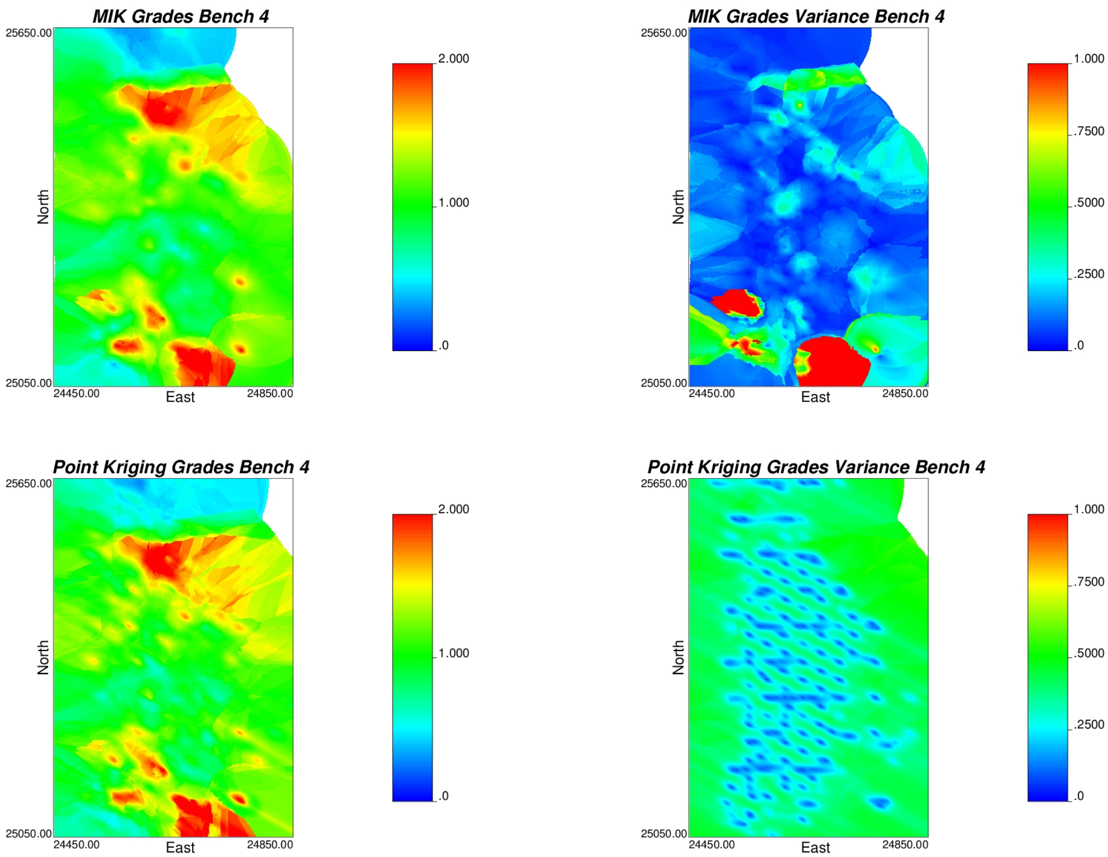

Figure 11: Maps for a representative planview of the MIK mean and variance (top) and the corresponding ordinary kriging results (bottom) for unit 20.

Method	Mean	Std. Dev.	Bias
Declustered distribution	1.186	0.658	–
Ordinary kriging	1.163	0.476	-1.9%
MGK (simple kriging)	1.146	0.385	-3.4%
MIK (ordinary kriging)	1.140	0.463	-3.9%

Table 6: Mean and standard deviation of declustered distribution and estimated points with ordinary kriging, multiGaussian kriging and multiple indicator kriging in unit 20.

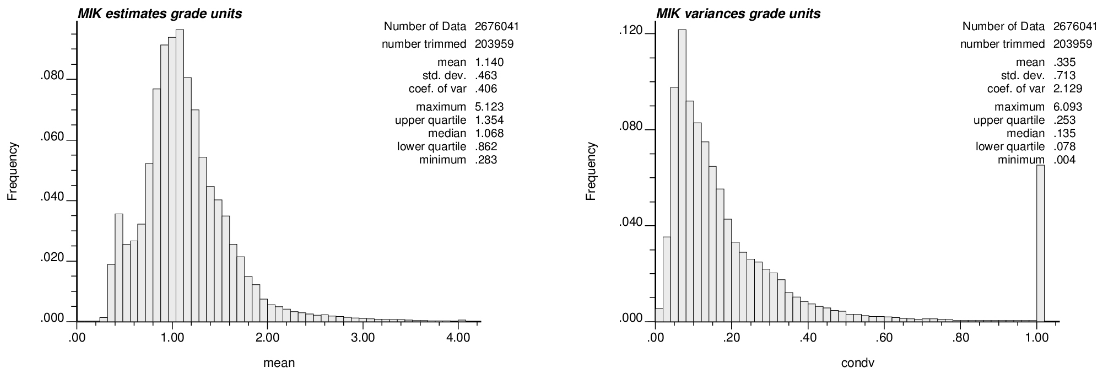

Figure 12: Histograms of the MIK mean and variance for unit 20.

Calibration

To show the sensitivity to the parameters of the tail extrapolation, a hyperbolic model is used with power 1.0 for the high tail. Results are displayed in **Figure 13**. The global bias is slightly reduced. If deemed necessary, further efforts to reduce the bias could be done.

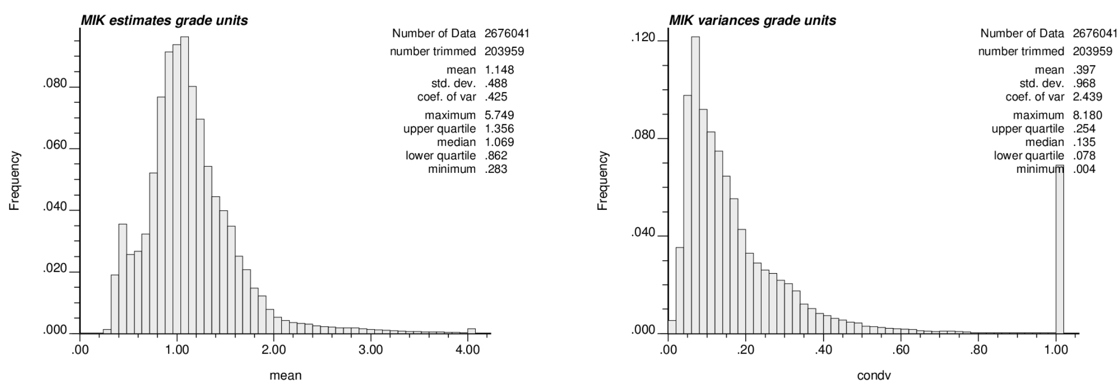

Figure 13: Histograms of the MIK mean and variance for unit 20, after changing tail extrapolation.

1.3 Comparison

To conclude this example, some comparisons are presented. **Figure 14** shows the scatter plots between estimates and between variances for MIK and MGK, and between MIK and OK. It is interesting to see the good match in the estimates, except for high grades, where ordinary kriging (in the Y axis) seems to give higher grades. Also, there is a cluster of points with clear differences around indicator estimates near 1%Cu that should be investigated. The relationship between variances is non-linear, as with MGK and with high dispersion. When comparing MIK and MGK (bottom scatter plots in the same figure), we can see again a good match in the estimates and some relation between the conditional variances. This can be explained by the fact that both methods model uncertainty differently, thus leading to different results. As both capture the proportional effect (**Figure 15**), some positive correlation is apparent in the variances.

1.4 Discussion

MultiGaussian kriging and multiple indicator kriging are two methods to assess the local point uncertainty. They rely on different assumptions therefore yield different results.

The main difference in assumption of the methods is that under the multiGaussian assumption, a single variogram model determines the behavior for all thresholds. In fact, this behavior is symmetric with respect to the median, thus, implicitly, in a multiGaussian model the indicator variogram at quantiles p is the same than the one obtained at a quantile $1-p$.

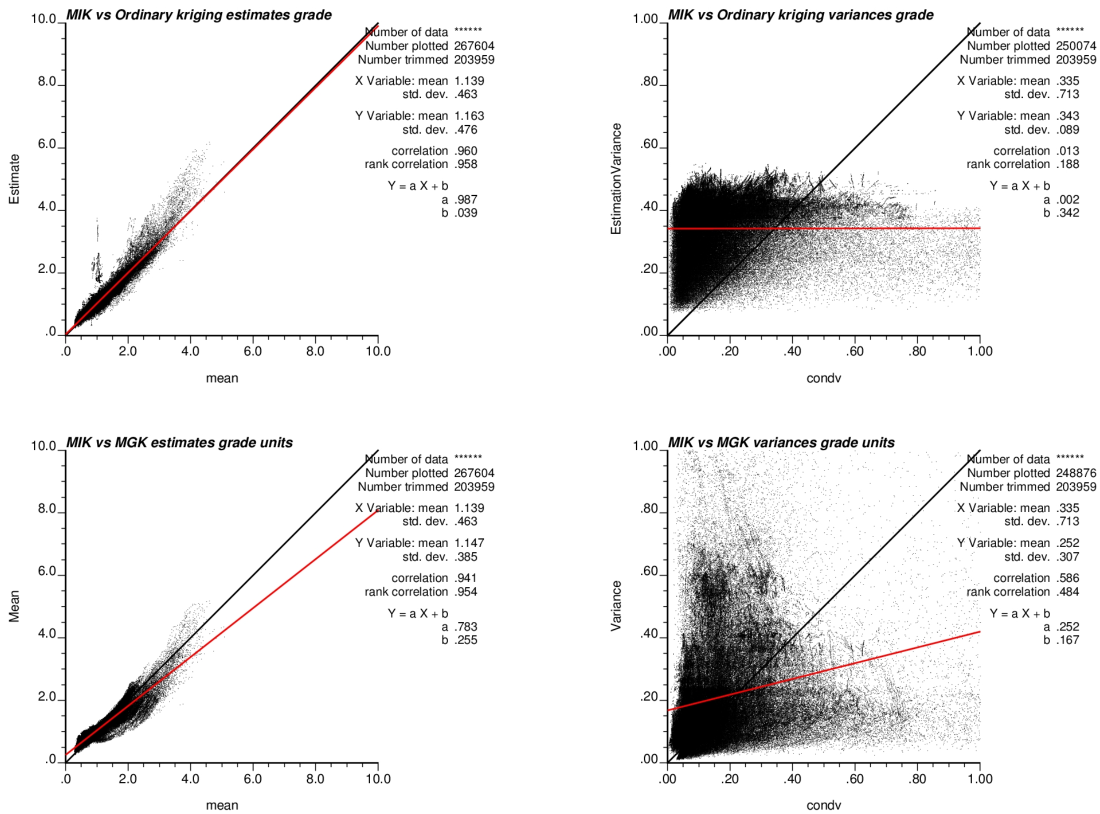

Figure 14: Scatter plots between estimates and variances for different methods.

In some applications this may seem unrealistic. For example, when the continuity of high permeability has a large ranges, while that of low permeability shows less correlation, then these thresholds should be modeled differently. In such a case, a multiGaussian assumption may be a poor choice, particularly if the high (or low) permeability continuity is critical for the model developed, as in the case of characterizing a possible nuclear waste repository.

In practice, multiGaussian kriging has seldom been used,

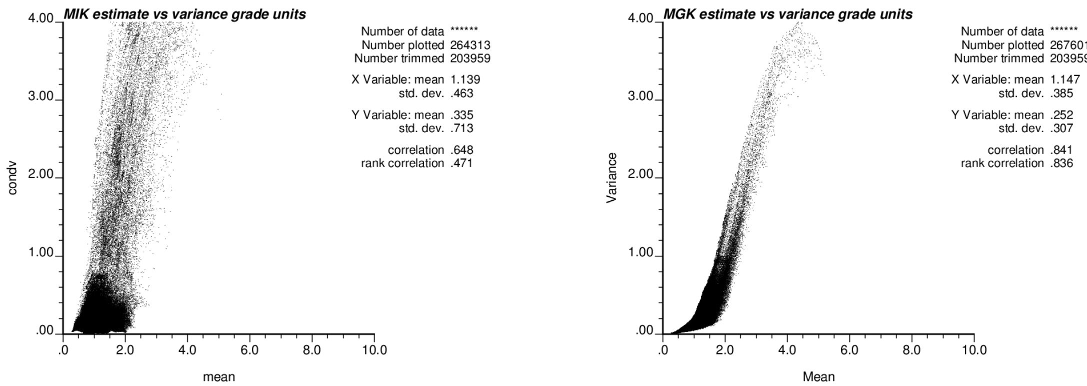

Figure 15: Comparison of proportional effect captured with MIK and MGK.

although its theoretical foundation is solid. Indicators, have been used to model grade distributions in precious metals deposits, but they suffer from many problems that require careful attention to many details.