Locally Stationary MultiGaussian Kriging with Local Change of Support Model

David F. Machuca-Mory and Clayton V. Deutsch

The incorporation of location-dependent distributions and statistics in multiGaussian kriging is proposed to overcome the limitations imposed by the strict stationarity assumption. These are obtained using distance weighting functions and are defined specifically for every location to be estimated. Local distributions require local Gaussian transformations. These are modeled using Hermite polynomial series, which are efficient and allow implementing the discrete Gaussian change of support model with locally varying parameters. Location dependent variogram models complement the definition of the location-dependent distributions and its statistics offering the capability of adjusting to local changes of the spatial continuity. The Locally Stationary multiGaussian Kriging algorithm uses the local Hermitian Gaussian transformation and local change of support model to produce point and block support estimates.

Introduction

Kriging within a Gaussian framework has been proposed since the early years of Geostatistics for problems where the local distribution rather than just a single estimated value is required (Matheron, 1976; Verly, 1983). Such problems are common in the mining industry, where ore and waste is selected relative to a cut-off, and the environmental fields, where the local risk of exceeding a permissible threshold needs to be evaluated. The idea is to transform the original data to a standard normal distribution and assume that the resultant multivariate distribution matches the multivariate Gaussian distribution (Deutsch & Journel, 1998). Under this assumption of multigaussianity, simple kriging provides the mean and variance of conditional distributions. The conditional cumulative distribution function (ccdf) is subsequently backtransformed in order to calculate the proportions above the given thresholds or the risk of exceeding them in original units.

MultiGaussian Kriging (MGK) is relatively easy to perform, but the use of MGK in practice has been limited due the restrictions imposed by simple kriging within a strictly stationary framework. To overcome this limitation, this paper proposes the implementation of multiGaussian Kriging under a locally, rather than globally, stationary assumption. Local stationarity requires of local cdfs and thus, local Gaussian transformations. Local measures of spatial continuity and their corresponding fitted models complement them and offer the capability of adjusting the estimation to local changes in the spatial continuity. These local distributions and statistics are obtained using smoothly changing distance weights in relation to reference points distributed within a domain. These local cdfs are locally transformed by normal scores transformation. Instead of keeping the complete transformation table, the local transformation functions are modelled by Hermite polynomial series. Besides being a more efficient way to store the transformation functions at different locations, using Hermite polynomials allows the implementation of a local discrete Gaussian change of support model (dgm). The local dgm allows incorporating local changes in the spatial continuity of the attribute when estimating at block support.

Previous papers have covered the issues concerning to the selection of the distance function and its parameters (Machuca-Mory & Deutsch, 2008a) , and the use of the resulting weights for inferring the local cdfs and their statistics, and for modelling the local transformation function using Hermite polynomial series (Machuca-Mory & Deutsch, 2008b). This paper focuses on the use of the local cdfs and their statistics in locally stationary estimation within the multiGaussian framework.

Locally Stationary MultiGaussian Point Kriging

The locally stationary simple kriging (LSSK) equations are similar to the traditional SK. The only difference is that the variogram model is updated at every location and, in the case of LSMGK, local transforms are used. The LSSK system is expressed as:

$$\sum_{\beta=1}^{n(\mathbf{o})} \lambda_{\beta}^{(LSSK)}(\mathbf{o})\rho(\mathbf{u}_{\beta}-\mathbf{u}_{\alpha};\mathbf{o}) = \rho(\mathbf{o}-\mathbf{u}_{\alpha};\mathbf{o}) \quad \alpha = 1,...,n(\mathbf{o}) \tag{1}$$

The LSSK estimation variance is given by:

$$\sigma^2_{LSSK}(\mathbf{o}) = C(0;\mathbf{o})\left[1 - \sum_{\alpha=1}^{n(\mathbf{o})} \lambda_\alpha^{(LSSK)}(\mathbf{o})\rho(\mathbf{o}-\mathbf{u}_\alpha;\mathbf{o})\right] \tag{2}$$

While the LSSK estimates is obtained from:

$$Z^*_{LSSK}(\mathbf{o}) = \sum_{\alpha=1}^{n(\mathbf{o})} \lambda_\alpha^{(LSSK)}(\mathbf{o})[Z(\mathbf{u}_\alpha)] + \left[1 - \sum_{\alpha=1}^{n(\mathbf{o})} \lambda_\alpha^{(LSSK)}(\mathbf{o})\right] m(\mathbf{o}) \tag{3}$$

The posterior ccdf in original units, $F(\mathbf{o}; z^*_p(\mathbf{o}) \mid n(\mathbf{o}))$ is built, by back-transforming a number of *P* quantiles $y^*_p(\mathbf{o})$ of the posterior ccdf in Gaussian units, $G'(\mathbf{o}; y^*_p(\mathbf{o}) \mid n(\mathbf{o}))$ with mean equal to the LSSK estimator Y^*_{LSSK} and standard deviation equal to the squared root of LSSK variance, $\sigma_{LSSK}(\mathbf{o})$:

$$z^*_p(\mathbf{o}) = \varphi_Z(y^*_p(\mathbf{o});\mathbf{o}) \simeq \sum_{q=0}^{Q} \phi_q(\mathbf{o}) H_q[y^*_p(\mathbf{o})] = \sum_{q=0}^{Q} \phi_q(\mathbf{o}) H_q[Y^*_{LSSK}(\mathbf{o}) + \sigma_{LSSK}(\mathbf{o}) \cdot t_p] \tag{4}$$

Where $F(\mathbf{o}; z^*_p(\mathbf{o}) \mid n(\mathbf{o})) = G'(\mathbf{o}; y^*_p(\mathbf{o}) \mid n(\mathbf{o})) = G(t_p) = p$, and $G(\bullet)$ and t_p are the standard Gaussian cdf and quantile, respectively. The location-dependent coefficients are obtained from the approximation of local Gaussian transformation by series of Hermite polynomials (Chilès & Delfiner, 1999). The estimator in original units can be obtained from the average of the $z^*_p(\mathbf{o})$ quantiles, given that their number P is big enough, in practice between 100 and 200:

$$Z^*_{LSMK}(\mathbf{o}) = E[z^*_p(\mathbf{o})] = E[\varphi_Z(y^*_p(\mathbf{o});\mathbf{o})] \simeq \frac{1}{P}\sum_{p=1}^{P}\sum_{q=0}^{Q} \phi_q(\mathbf{o}) H_q[Y^*_{LSSK}(\mathbf{o}) + \sigma_{LSSK}(\mathbf{o}) \cdot t_p] \tag{5}$$

Locally Stationary MultiGaussian Block Kriging

When working within the multiGaussian framework, block estimates in original units require a change of support model. The local normal scores transformation function and the local variogram model can be assumed constant within the block volume *v*(**o**), if it is relatively small compared with the entire domain. Thus, any randomly located sample within the volume centred at **o** is transformed by the same function:

$$Z(\mathbf{o}_i) = \varphi(Y(\mathbf{o}_i);\mathbf{o}) \qquad \forall \mathbf{o}_i \in v(\mathbf{o}) \tag{6}$$

The block grade can be estimated as the average of *M* point estimates within the block. Therefore, the posterior block support ccdf can be built for *P* cut-offs z_p, p=1,…,P, from (Chilès & Delfiner, 1999):

$$\begin{aligned} F_v(\mathbf{o}; z_p \mid n(\mathbf{o})) &\simeq \text{Prob}\left\{\frac{1}{M}\sum_{i=1}^{M} Z(\mathbf{o}_i) \le z_p \mid Z(\mathbf{u}_\alpha) : \alpha = 1,\dots,n(\mathbf{o})\right\} \\ &= \text{Prob}\left\{\sum_{i=1}^{M} \varphi\big(Y(\mathbf{o}_i);\mathbf{o}\big) \le M \cdot z_p \mid Y(\mathbf{u}_\alpha) : \alpha = 1,\dots,n(\mathbf{o})\right\} \\ &= E\left[I\left(\sum_{i=1}^{M} \varphi\big(Y(\mathbf{o}_i);\mathbf{o}\big); M \cdot z_p\right) \mid Y(\mathbf{u}_\alpha) : \alpha = 1,\dots,n(\mathbf{o})\right] \end{aligned} \tag{7}$$

Where $I[\bullet]$ is the indicator function, which takes a value of one if the cutoff z_p, and zero, otherwise. In Gaussian space, the ccdf's at the locations $\mathbf{o}_i$ are fully defined by the SK estimate and variance. Therefore, the posterior block support ccdf can be obtained from (Emery, 2006):

$$F_v(\mathbf{o}; z_p \mid n(\mathbf{o})) = \int I\left[\sum_{i=1}^{M} \varphi\Big(Y^*_{LSSK}(\mathbf{o}_i) + \sigma_{LSSK}(\mathbf{o}_i) \cdot t;\mathbf{o}\Big); M \cdot z_p\right] g(t)\,dt \tag{8}$$

This expression is calculated numerically by drawing a large number *N* of standard Gaussian distributed random numbers, and averaging the results (Verly, 1984):

$$F_v(\mathbf{o};z_p \mid n(\mathbf{o})) \simeq \frac{1}{N}\sum_{j=1}^{N} I\left[\sum_{i=1}^{M}\varphi\Big(Y^*_{LSSK}(\mathbf{o}_i)+\sigma_{LSSK}(\mathbf{o}_i)\cdot t_j;\mathbf{o}\Big);M\cdot z_p\right] \tag{9}$$

Building the complete block support ccdf requires this numerical calculation for different cut-offs. Thus, this approach may be computationally demanding if the block support ccdf is required in detail. A more efficient approach is given by the Discrete Gaussian Model. For this change of support model, the point support RVs are considered randomly located at points $\underline{\mathbf{o}}$ within the blocks. The point and block support Gaussian transformed RVs $Y(\underline{\mathbf{o}})$ and $Y_v(\mathbf{o})$ are assumed bigaussian with location-dependent correlation $r(\mathbf{o})$. The Gaussian transformation functions for both variables are given by (Emery, 2005):

$$\begin{cases} Z(\underline{\mathbf{o}})=\varphi(Y(\underline{\mathbf{o}});\mathbf{o}) \quad = \displaystyle\sum_{q=0}^{Q}\phi_q(\mathbf{o})H_q\left(Y(\underline{\mathbf{o}})\right) \\ Z_v(\mathbf{o})=\varphi_v(Y_v(\mathbf{o});\mathbf{o})=\displaystyle\sum_{q=0}^{Q}\phi_q(\mathbf{o})r^q(\mathbf{o})H_q\left(Y_v(\mathbf{o})\right) \end{cases} \tag{10}$$

Where the location-dependent change of support coefficient $r(\mathbf{o})$ is obtained from (Rivorairdd, 1991):

$$\mathrm{var}[Z_v(\mathbf{o})]=\gamma_Z(\infty;\mathbf{o})-\frac{1}{M^2}\sum_{i=1}^{M}\sum_{j=1}^{M}\gamma_Z(\mathbf{o}_i-\mathbf{o}_j;\mathbf{o})=\sum_{q=1}^{Q}\phi_q^2(\mathbf{o})r^{2q}(\mathbf{o}) \tag{11}$$

With $\gamma_Z(\mathbf{h};\mathbf{o})$ as the non-standardized variogram in original units for the location **o**. Working with correlograms instead of variograms is desirable because the greater stability and more direct interpretation of the former, in this case the expression (4.16) is equivalent to:

$$\mathrm{var}[Z_v(\mathbf{o})]=C_Z(0;\mathbf{o})\left(1-\frac{1}{M^2}\sum_{i=1}^{M}\sum_{j=1}^{M}\Big[1-\rho_Z(\mathbf{o}_i-\mathbf{o}_j;\mathbf{o})\Big]\right)=\sum_{q=1}^{Q}\phi_q^2(\mathbf{o})r^{2q}(\mathbf{o}) \tag{12}$$

The experimental location-dependent correlograms, calculated from normal scores transformed values are usually more stable than those in original units and, thus, easier to model. Therefore, it is preferred to calculate and model these measures of spatial correlation on the transformed values and then back-transform them to original units. This assures the consistency between the correlograms used in LSMK and those in original units. The back-transformation of the normal scores correlograms is achieved by considering the relationship between the covariances in normal scores, $C_Y(\mathbf{h};\mathbf{o})$, and original units, $C_Z(\mathbf{h};\mathbf{o})$. This is given by (Guibal, 1987):

$$C_Z(\mathbf{h};\mathbf{o})=\sum_{q=1}^{Q}\phi_q^2(\mathbf{o})\big[C_Y(\mathbf{h};\mathbf{o})\big]^q \tag{13}$$

Alternatively, if location-dependent variograms are used, the local variogram value in original units is approximated by:

$$\gamma_Z(\mathbf{h};\mathbf{o})=\sum_{q=1}^{Q}\phi_q^2(\mathbf{o})\Big[1-\big(1-\gamma_Y(\mathbf{h};\mathbf{o})\big)^q\Big] \tag{14}$$

In practice, the location-dependent change of support coefficient is calculated only at the anchor point locations and subsequently interpolated between them. Counting with all the required parameters the block support posterior ccdf is built for different $z_p^*(v(\mathbf{o}))$ quantiles by:

$$\begin{aligned} z_p^*(v(\mathbf{o})) = \varphi_v(y_p^*(v(\mathbf{o}));\mathbf{o}) &= \sum_{q=0}^{Q}\phi_q(\mathbf{o})\cdot r^q(\mathbf{o})\cdot H_q[y_p^*(v(\mathbf{o}))] \\ &= \sum_{q=0}^{Q}\phi_q(\mathbf{o})\cdot r^q(\mathbf{o})\cdot H_q[Y^*_{LSSK}(v(\mathbf{o}))+\sigma_{LSSK}(v(\mathbf{o}))\cdot t_p] \end{aligned} \tag{15}$$

As in (5), the estimate at block support is approximated numerically by the average of the *P* $z_p^*(v(\mathbf{o}))$ quantiles, provided that *P* is big enough. Deriving the probability of exceeding certain threshold is straightforward once the complete distribution in original units has been defined.

Implementation

The FORTRAN program kt3d_lMG implements the methodology presented above. Figure 1 presents the format for the required parameter file. The input file contains the data values in original units. Since spikes in data may cause numerical inconsistencies in the fitting of the local transformation function, it is recommended to modify the data values using the program DESPIKE first. The local coefficients for the Hermitian Gaussian transformation model, as well as the local variogram model parameter, are provided in Gslib type grid files of the same dimensions as the estimation grid.

At each block in the grid the program reads the Hermite coefficients and local variogram parameters. The local transformation table is reconstructed for 200 Gaussian distributed quantiles. After the correction of order relation problems, the local normal scores transforms of the original data values are obtained by interpolating the immediate lower and upper quantiles in Gaussian units. Figure 2, left, shows a 1-D dataset corresponding to the silver grades obtained from a hole drilled at a South American sulfide deposit. The right side of the same figure shows, for the same dataset, the global and some local transformation functions along with their fit by Hermite polynomial series. Notice that the Hermite model fitted using a limited number of polynomials doesn't yield to an exact reproduction of the transformation function, but deviations are generally within tolerable ranges. Figure 3 presents the local nugget effect and variogram range of the exponential variogram models fitted on the local experimental values of the function 1-$\rho(\mathrm{h},\mathbf{o})$.

For the sake of clarity, point support MGK and LSMGK was performed at nodes shifted from the data locations, since, due to the exact interpolation property of kriging, spikes appear in the estimates and estimation variance curves at node locations. As it can be observed in Figure 4, left, MGK and LSMGK estimates are very similar when data is abundant. Contrarily, in less densely sampled areas MGK estimates tend to the global mean, while LSMGK approaches the local mean. Other differences in the local variability of estimates can be explained by the use of variogram models with locally varying parameters. Differences between the estimation variances in original units of MGK and LSMGK are greater (see Figure 4, right).

The local prior variance has a major impact in the LSMGK estimation variance, while low local nugget effect and long local ranges translate in lower LSMGK estimation variances. The prior point-support local variance is obtained from the sum of square local Hermite coefficients, such as in expression (11) and with r =1. The change of support coefficient is obtained by iterating the last term of expression (12) using different values for r until the value of the block support variance calculated from the average variogram is approximated within a tolerance. The variogram values in original units are backtransformed from the local variogram in normal units using equation (14). Figure 5, left, shows the prior local point-support variances approximated from the sum of square local Hermite coefficients and the prior block-support variances obtained from expression (12). The global and local change of support coefficients are presented in the right side of Figure 5. The change of support coefficient is affected mainly by the nugget effect and the variogram range, in that order. The use of a locally varying nugget effect allows imparting different degrees of smoothing of the block support distribution depending on the local variability informed by local variograms. Thus, the LSMGK block support estimates (left side of Figure 6) may appear smoother than MGK block support estimates in areas where the change of support coefficient is low and more variable when it is high. As in the point support case, the block support LSMGK estimation variances are affected mostly by the variance values of the prior local distributions (right side of Figure 6).

2D example

A 2-D comparison between MGK and LSMGK for block support estimation is presented using the Walker Lake Data set. Figure 7 shows a map of the clustered point samples over the "true" reference values averaged in blocks of 10 x 10 units. The location-dependent distributions and their statistics were obtained in an anchor point grid of 20 x 20 units using a Gaussian kernel with a bandwidth of 20 units as distance weighting function. The local transformation functions were modelled at each anchor point location and the resulting Hermite coefficients were interpolated at each block centre. The same interpolation was applied to the parameters of the local variogram models fitted on the location-dependent experimental correlograms calculated using the normal scores transform of the clustered dataset. Figure 8 shows maps of the local variogram model parameters at the block scale. In the same figure, the marks at the left side of the colour legends indicate the parameters of the global variogram model. For this case, most of the variations of the local variogram parameters can be visually related to patterns in the data values. Compare, particularly, the local anisotropy orientations with Figure 7.

Figure 9 shows the estimates and variances at block size after backtransforming the distributions in Gaussian space using a transformation function modified by the discrete Gaussian change of support model. The use of a single variogram imparts a uniform spatial distribution to the MGK estimates, while the estimation variances responds to changes in the data configuration as well as in the local variability. Block LSMGK estimates (Figure 10, left) show a better continuity of low and grade zones, more similar to the reference dataset. The estimation variances (Figure 10, right) respond not only to changes in the local data configuration and variability, but also in the local spatial continuity informed by the variogram.

The improved reproduction of non-stationary features translates in a better ore/waste classification. For this example, the LSMGK grade-tonnage curves (Figure 11, left) show a lower overestimation of the low-grade material and a slight reduction in the underestimation of high-grade material. In general, the grade-tonnage curves for LSMGK are closer to the reference curves than the MGK curves. A reduced ore/waste misclassification leads to improved outputs of the transfer functions, such as the profit function. A simplified form of the profit as a function of a cut-off *z* is used in this paper; this is expressed as (Journel & Kyriakidis, 2004):

$$P(z) = K(z) \cdot \big(Q(z) - z \cdot T(z)\big) - K_0 \tag{16}$$

With $Q(z)$ and $T(z)$ as the effective quantity of metal and tonnage recovered by classifying the blocks according their estimate value in relation to the cut-off z, while $K(z)$ and K_0 are the variable and fixed mining costs. K_0 was fixed to a value of 200, and the variable costs were modelled in function of the cut-off as:

$$K(z) = -1.98\times10^{-10} z^2 + 4.25\times10^{-7} z + 1.25\times10^{-5}$$

At low cut-off values, the effective profit obtained by classifying the blocks according to the LSMGK estimates is higher than the obtained using MGK (see Figure 11, right) indicating a lower ore/waste misclassification for the locally stationary technique. At higher cut-offs the profit derived from LSMGK and MGK estimates converge to the actual profit, indicating for this example that both methods yield a correct classification above a threshold of 400.

Conclusions

Locally stationary multiGaussian kriging is a viable alternative to traditional multiGaussian approach, which is constrained by the restrictions imposed by the assumption of strict stationarity. Using distance weighted distributions and statistics allows adapting to changes in the local mean, variance, histogram shape and spatial continuity. The modelling of local transformation functions by means of Hermite polynomials series is a compact alternative to the use of local transformation tables, and allows the implementation of a discrete Gaussian change of support model with locally varying parameter. The Hermite model may introduce small errors in the Gaussian transformation, particularly at the extremes of the distribution, but these are generally tolerable. Moreover, the flexibility provided by the incorporation of location-dependent statistics can improve the ore-waste classification and hence the performance of transfer functions that depend of it.

References

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```
                  Parameters for KT3D_1MG
                  ***********************

START OF PARAMETERS:
example.dat                  - file with data
0  2  3  4  12  0            - columns for DH,X,Y,Z,var,sec var
-10.0   1.0e21               - trimming limits
LocalHerpol.dbg              - file with local Hermite polynomials (in columns)
36 7                         - number of hermite polynomials and column for phi(0)
0.1                          - acceptable error for block variance
1   26                       - minimum and maximum value in original units
0                            - option: 0=grid, 1=cross, 2=jackknife
xvk.dat                      - file with jackknife data
1   2   0    3    0          - columns for X,Y,Z,vr and sec var
1                            - debugging level: 0,1,2,3
MGkt3d-loc-blk.dbg           - file for debugging output
MGkt3d-loc-blk.out           - file for kriged output
100   2.0  4.0               - nx,xmn,xsiz
100   2.0  4.0               - ny,ymn,ysiz
100  -398   4.0              - nz,zmn,zsiz
1    1      2                - x,y and z block discretization
2    16                      - min, max data for kriging
0                            - max per octant (0-> not used)
65.0   65.0  65.0            - maximum search radii
 0.0   0.0   0.0             - angles for search ellipsoid
0      0.000                 - 0=SK,1=OK,2=non-st SK,3=exdrift
0 0 0 0 0 0 0 0 0            - drift: x,y,z,xx,yy,zz,xy,xz,zy
0                            - 0, variable; 1, estimate tren
extdrift.dat                 - gridded file with drift/mean
0                            - column number in gridded file
1    0.41  1.0               - nst, nugget effect
2    0.59  0.0   0.0   0.0   - it,cc,ang1,ang2,ang3
         21.0  21.0  21.0    - a_hmax, a_hmin, a_vert
lC0.out                      - Local nugget effect (same grid)
exp.out                      - Local exponent of the stable model (required if it =6)
lCC.out                      - Local sill for 1st structure
lhmax.out                    - Local maximum range for 1st structure
lhmin.out                    - Local minimum range for 1st structure
lhver.out                    - Local vertical range for 1st structure
ang1_1.out                   - Local angle 1 for 1st structure
ang2_1.out                   - Local angle 2 for 1st structure
ang3_1.out                   - Local angle 3 for 1st structure
c2.out                       - Local sill for 2nd structure
hmax2.out                    - Local maximum range for 2nd structure
hmin2.out                    - Local minimum range for 2nd structure
hmin2.out                    - Local vertical range for 2nd structure
ang1_2.out                   - Local angle 1 for 2nd structure
ang2_2.out                   - Local angle 2 for 2nd structure
ang3_2.out                   - Local angle 3 for 2nd structure
```

Figure 1: Parameter file for the locally stationary multiGaussian kriging program

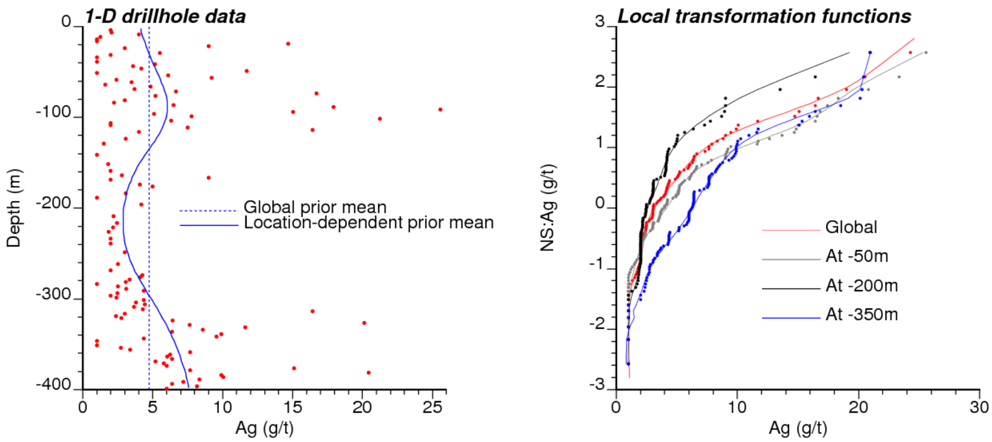

Figure 2: Left, Silver assays in a drillhole along with its global and local means. Right, global and three local transformation functions fitted using Hermite polynomial series.

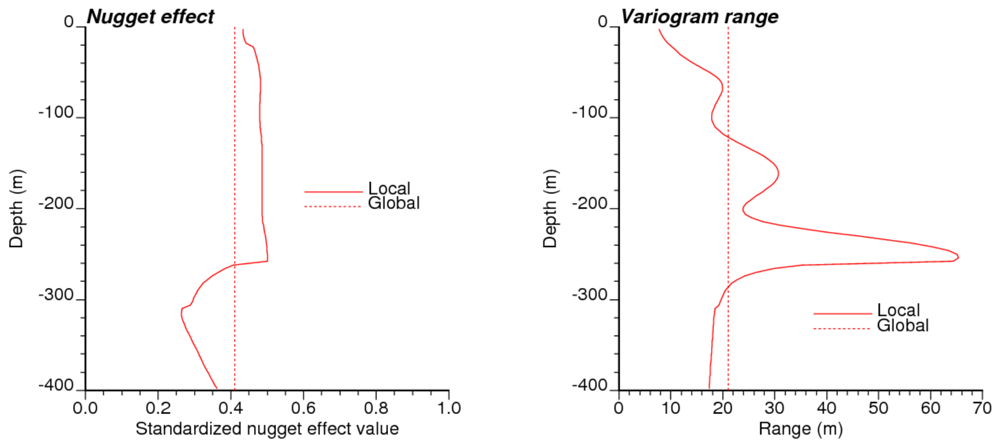

Figure 3: Local nugget effect (left) and range (right) fitted to the experimental local correlograms of the drillhole silver grades.

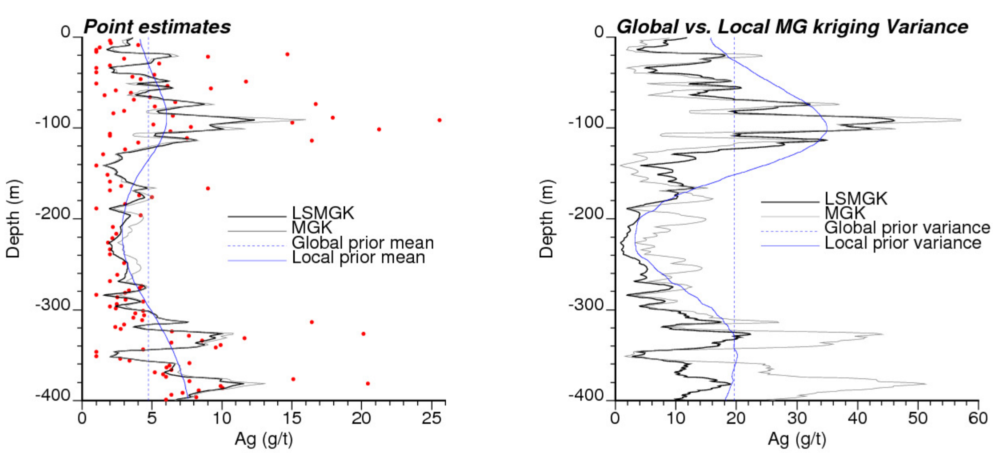

Figure 4: MGK and LSMGK estimates (left) and variances (right). The estimation nodes were shifted apart from the samples locations in order to avoid showing the spikes that appear due to the kriging property of exact interpolation.

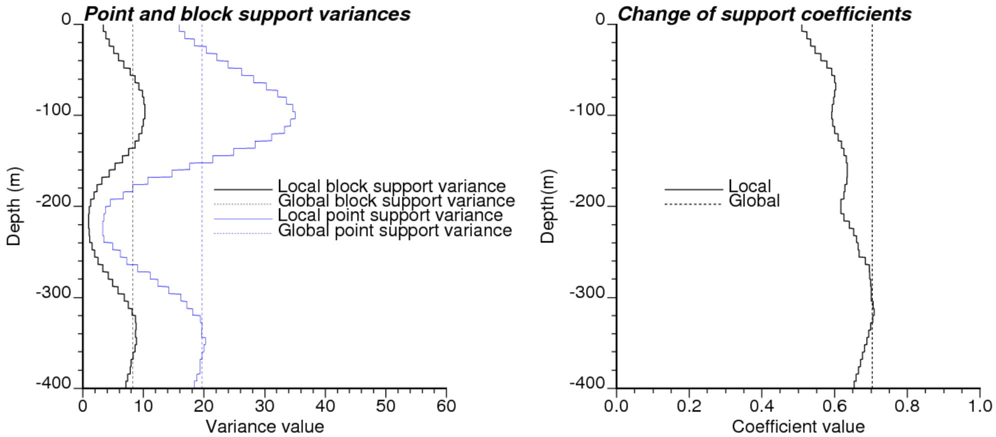

Figure 5: Point and block support prior local variances (left) and local change of support coefficients (right) inferred on the drillhole silver grades.

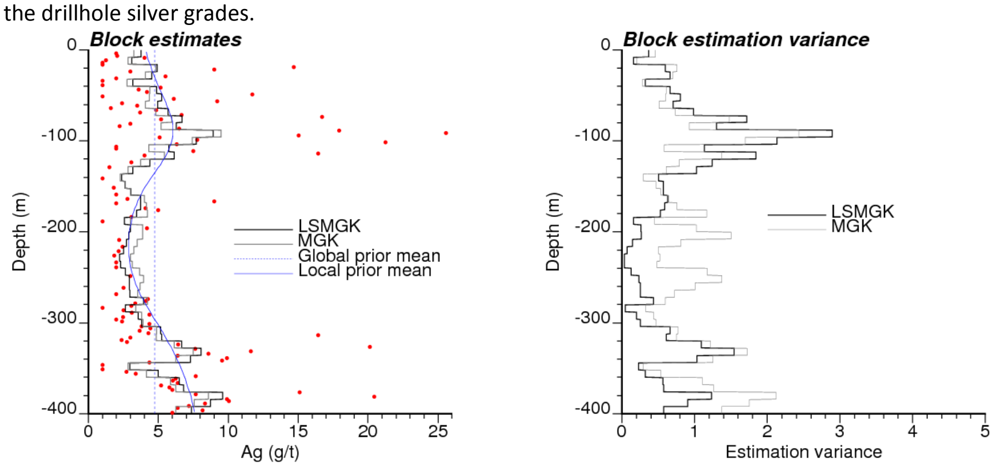

Figure 6: MGK and LSMGK block estimates (left). MGK and LSMGK block variances (right).

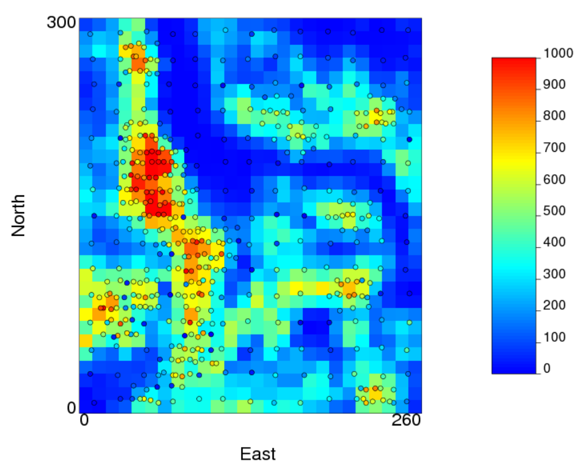

Figure 7: Point samples overlying the reference Walker Lake dataset blocked at 10 x 10 units.

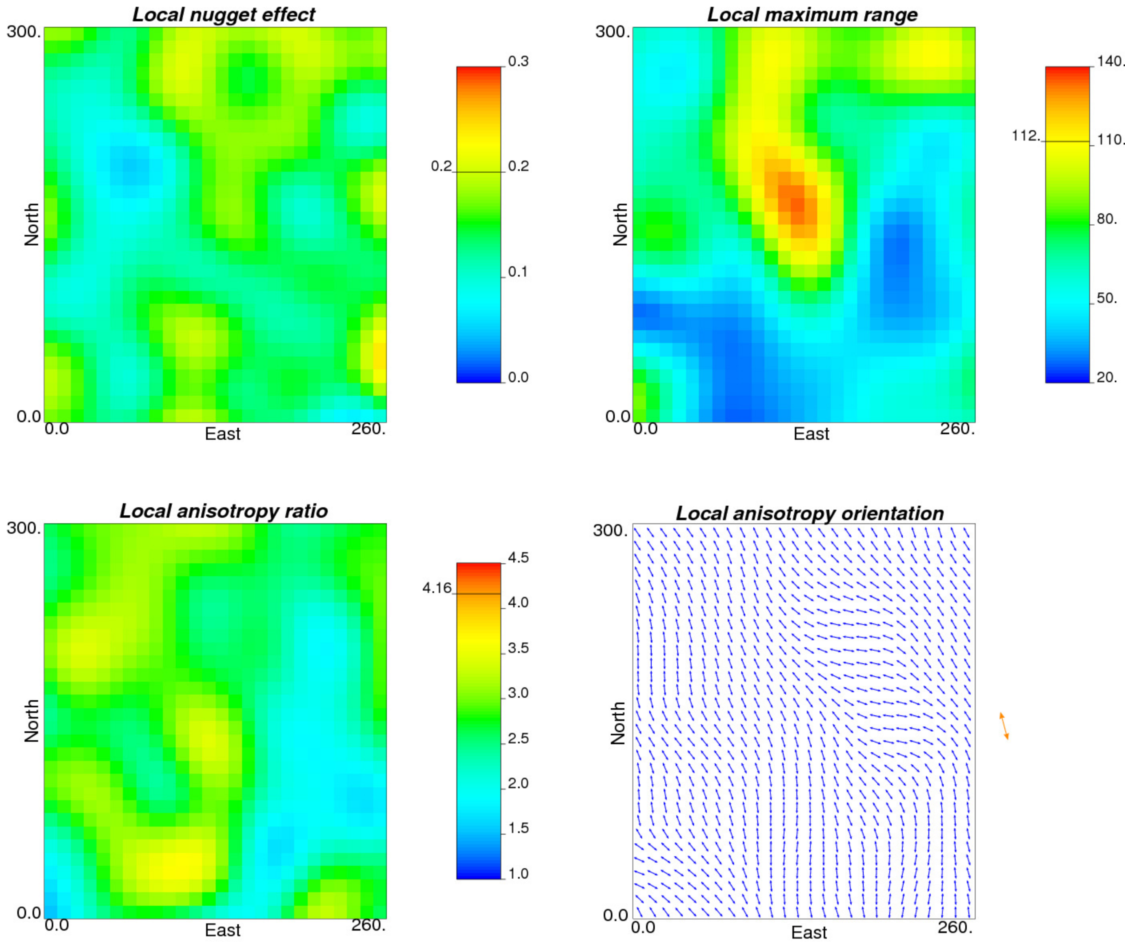

Figure 8: Local variogram parameters fitted on the local experimental correlograms calculated on the clustered Walker Lake dataset.

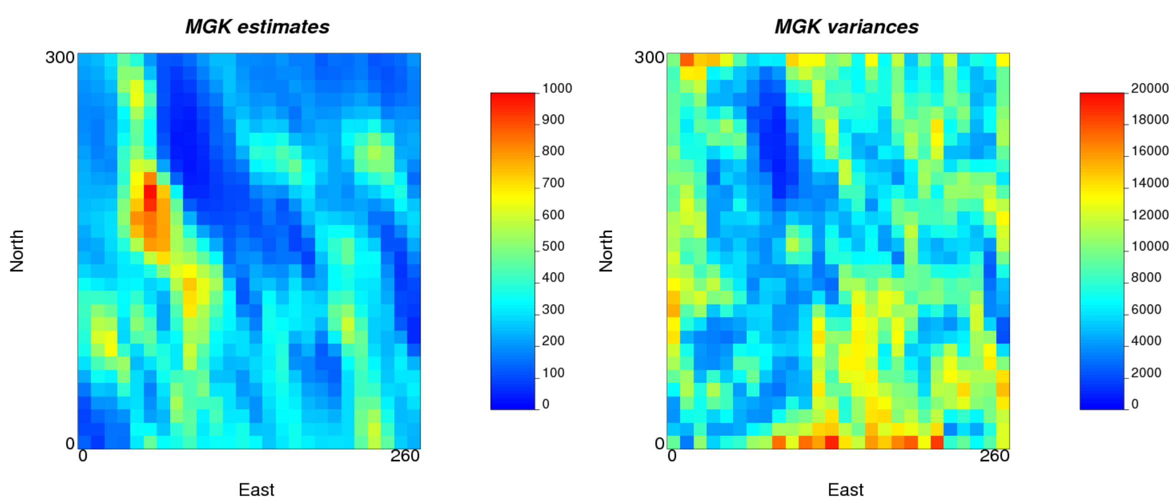

Figure 9: Traditional multiGaussian Kriging block estimates (left) and variances (right).

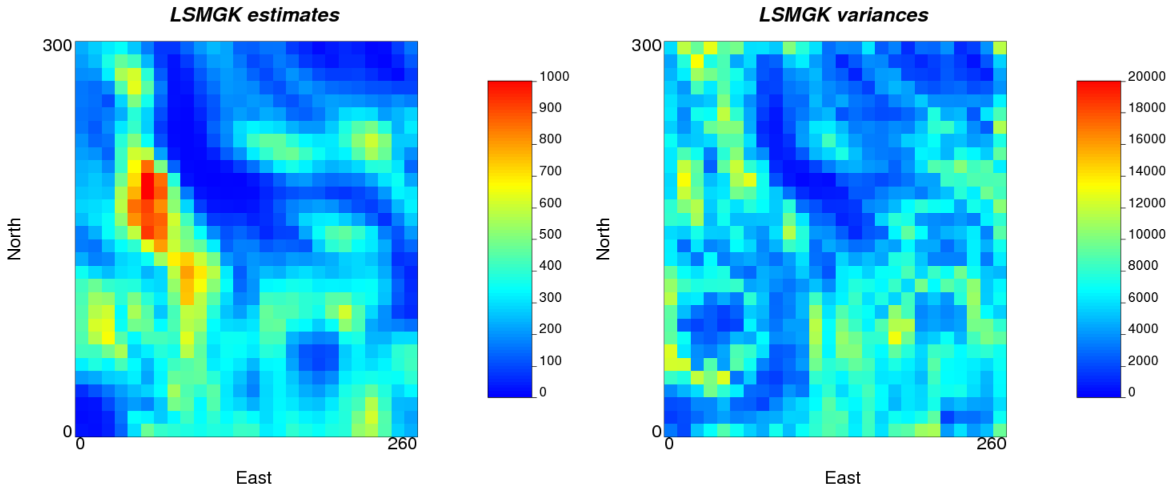

Figure 10: Locally stationary multiGaussian block estimates (left) and variances (right).

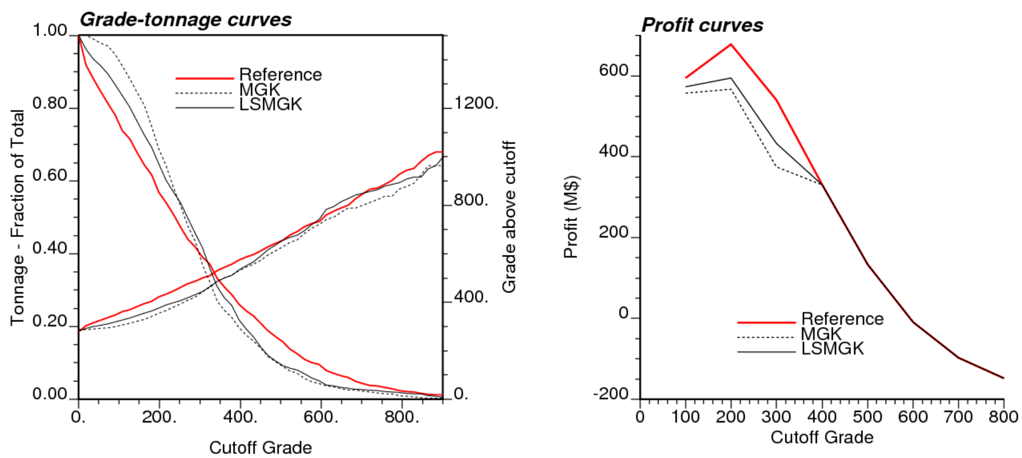

Figure 11: Grade tonnage curves (left) and profit function curves (right) for the reference exhaustive data (red line), MGK (dashed line) and LSMGK (solid black line).