Joint Fitting of Local Variograms in Non-stationary Geostatistics

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Locally weighted experimental measures of spatial continuity are calculated at multiple locations. Fitting the local variogram models require of a semiautomatic algorithm. Previous algorithms are based on the iterative minimization of an objective function defined as the mean square error between the experimental points and the variogram model curve. Sequential independent fitting of these local experimental 2-point statistics often produce locally anomalous parameter values and other discontinuities which are not coherent with the smoothly changing local statistics. An algorithm `globfit` for the joint fitting of the local variogram models at multiple anchor points is proposed. This algorithm uses spatial correlated random values for the iterative alteration of the globally stationary variogram model parameters, controls the occurrence of locally anomalous variogram parameter values and penalizes the parameter values that exceed thresholds defined by the user. The resulting local variogram model parameters change smoothly and allow the minimization of the mean square error within predefined constraints.

1. Introduction

Locally weighted measures of spatial continuity have been proposed for capturing the non-stationary features of spatial continuity (Machuca-Mory & Deutsch 2008b). These 2-point statistics are calculated at multiple anchor points within a domain. At each anchor point, data is weighted inversely proportional to their distance to such point using a smoothly decaying distance weighting function, such as the Gaussian kernel. The weight of a pair of samples is obtained by the geometric average of the weights assigned to the individual samples. These 2-point weights are incorporated in the traditional expression for the variogram, covariance and correlograms. If the weighting kernel bandwidth is wider than the average data spacing, the resulting location-dependent experimental measures of spatial correlation vary smoothly from one anchor point to another.

These location-dependent measures of spatial continuity are calculated for several directions at each anchor point. Since the number of required anchor points within a domain usually is in the range of few hundreds, the fitting of the corresponding local variogram models is only feasible with the help of a semiautomatic fitting algorithm. The program `varfit` (Larrondo et al. 2003) has been developed for the semiautomatic fitting of global variograms. As `varfit`, the variogram fitting algorithm implemented in this program is based on the iterative minimization of the average square error between the experimental variogram points and the proposed variogram model curve. `varfit` program can be easily modified to perform the sequential fitting of the location-dependent variograms going from an anchor point to the next. The local variogram model parameters, such as the nugget effect, the orientations and ranges of spatial continuity and others, obtained from the sequential independent fitting of local 2-point statistics tend to reflect diverse aspects in the non-stationarity in the spatial continuity. However, issues related to the individual fitting of the models and to the lack of strong constraints on the range of allowable parameter values are common. When local variogram fitting is performed at each anchor point independently of the models fitted at surrounding locations a common problem is the occurrence of isolated very low or very high parameter values and abrupt breaks in the continuity of the local variogram model parameters. These unwarranted discontinuities in the local variogram model parameters normally do not correspond to the smoothly changing location-dependent measures of spatial continuity within a domain. They usually happen when the local experimental variograms are very discontinuous, or they present a hole effect not taken into account by the variogram model. Figure 1 shows two location-dependent experimental variograms obtained at very close locations (0,0,-15) and (0,0,-16). They are practically the same, but their respective variogram models fitted independently are very different.

The same discontinuities that cause the abrupt variations in the local variogram model parameters may cause the fitting of fitting of unreasonably very high or very low parameter values Thus, the incorporation of user defined constraints is necessary for avoiding the occurrence of anomalous local parameter values. These constraints can be defined in relation to the geological knowledge available.

To avoid these and other issues the conjoint, rather than individual, semiautomatic fitting of multiple location-dependent variogram models is proposed. The algorithm implemented in the program `globfit`, uses spatially correlated random alterations for the recursive modification of the variogram model parameters and the occurrence of locally anomalous parameter values. Additionally, the program penalizes the parameter values that exceed an allowable range predefined by the user, minimizes the importance of the experimental local variogram points calculated with far sample pairs, and allows the incorporation of geological information on the local directions of continuity.

The main features implemented in the proposed algorithm are described in the next section. A 1-D dataset is used for illustrating the performance of the modified algorithm. Although the proposed algorithm requires more testing, the results so far show that the fitted local variogram model parameters change smoothly and coherently with the experimental location-dependent variograms.

2. Fitting Criteria for Location-Dependent Variogram Models

The main criteria for fitting a series of local variogram models is twofold: (1) The minimization of the mean square differences between the local experimental variograms and their corresponding proposed models, and (2) the consistency between model parameters fitted at contiguous anchor points. Both must be accomplished within user-defined tolerance ranges for the parameter values.

Least squares error minimization

The least-squares criterion for the fitting of variogram models has been proposed since the initial years of computational Geostatistics (David 1977, p.119). Weighted least-squares criteria (Cressie 1985; Goovaerts 1997) has been commonly adopted to account for the importance given to experimental points. The weights assigned to the experimental variogram points can be directly proportional to the quantity of information used for their inference or inversely proportional to the lag distance. The information used in the inference of the experimental points is quantified by the sum of the 2-point weights assigned to the pairs involved. Thus a weighting criterion, λ_{inf}, related to the information available is defined as:

$$\lambda_{\text{inf}}(\mathbf{h}_j,\mathbf{o})=\frac{\sum_{\alpha=1}^{N(\mathbf{h}_j)}\omega(\mathbf{u}_\alpha,\mathbf{u}_\alpha+\mathbf{h}_j;\mathbf{o})}{\sum_{j=1}^{n_{\text{exp.points}}}\sum_{\alpha=1}^{N(\mathbf{h}_j)}\omega(\mathbf{u}_\alpha,\mathbf{u}_\alpha+\mathbf{h}_j;\mathbf{o})} \tag{1}$$

$N(\mathbf{h}_j)$ is the number of pairs used to calculate the experimental point at the distance and orientation corresponding to $\mathbf{h}_j$. $\omega(\mathbf{u}_\alpha,\mathbf{u}_\alpha+\mathbf{h}_j;\mathbf{o})$ are the 2-point weights assigned to a pair of samples located at $\mathbf{u}_\alpha$ and $\mathbf{u}_\alpha+\mathbf{h}_j$ in relation to anchor point **o**. $n_{\text{exp.points}}$ is equal to the total number of experimental points calculated at different directions and for different lag distances. Another weighting criterion deals with the importance of experimental points for depicting the short scale continuity. The corresponding weights $\lambda_{dist}(\mathbf{h}_k)$ are calculated as the inverse of the lag distance $|\mathbf{h}|=h$ (Zhang et al. 1995; Larrondo et al. 2003):

$$\lambda_{dist}(\mathbf{h}_k)=\frac{\frac{1}{h_k}}{\sum_{k=1}^{n_{\text{exp.points}}}\frac{1}{h_k}} \tag{2}$$

In order to prevent the parameters from taking values that largely exceed the limits judged as reasonable by the user a penalty function is considered. The penalty function can take different forms; this one is a simple quadratic function. Thus if a number n_{par} of local variogram parameters, $b_\beta(\mathbf{o}),\ \beta=1,...n_{par}$, is to be controlled rather than fixed, a penalty is applied to those values, that exceed a range $(b_{\beta,\min},b_{\beta,\max})$ imposed by the user:

$$W_\beta\left(b_\beta(\mathbf{o})\right)=\begin{cases}k\cdot(b_\beta(\mathbf{o})-b_{\beta,\min})^2 & \text{if } \ b_\beta(\mathbf{o})\le b_{\beta,\min}\\ 0 & \text{if } \ b_{\beta,\min}<b_\beta(\mathbf{o})<b_{\beta,\max}\\ k\cdot(b_\beta(\mathbf{o})-b_{\beta,\max})^2 & \text{if } \ b_\beta(\mathbf{o})\ge b_{\beta,\max}\end{cases} \tag{3}$$

The factor *k* controls the strength of the penalty. The higher this value is, the harder is for the algorithm to produce local variogram parameters that exceed the predefined range. Usually, a penalty factor higher than one avoids the occurrence of parameter values beyond the range $(b_{\beta,\min}, b_{\beta,\max})$. A penalty factor smaller than one can be used if the practitioner decides to allow some flexibility in the parameter limits, and thus, to avoid the hard capping of the parameter values. The minimum and maximum allowable parameter values can be set as absolute or as relative tolerances to previously defined local values. The second form can be useful for allowing a certain degree of flexibility in the fitting of local anisotropy angles guided by values taken from field measurements or the geological interpretation of the deposit.

Thus, given an experimental spatial correlation measure, $\hat{\gamma}(\mathbf{h};\mathbf{o})$, and the proposed model value at the same lag **h**, $\gamma(\mathbf{h};\mathbf{o})$, the optimization criterion for semi-automatic fitting of the local variogram at an anchor point **o** is to minimize the next objective function:

$$O(\mathbf{o})=\frac{1}{n_{\text{exp.points}}}\sum_{j=1}^{n_{\text{exp.points}}}\lambda(\mathbf{h}_j,\mathbf{o})\left(\gamma(\mathbf{h}_j;\mathbf{o})-\hat{\gamma}(\mathbf{h}_j;\mathbf{o})\right)^2+\frac{1}{n_{\text{par}}}\sum_{\beta=1}^{n_{\text{par}}}W_\beta\left(b_\beta(\mathbf{o})\right) \tag{4}$$

The weights $\lambda(\mathbf{h}_j,\mathbf{o})$ can take the form of either Expression (1) or (2) or they can be built as the product of both. The penalties $W_\beta\left(b_\beta(\mathbf{o})\right)$ are as in Expression (4). This minimization criterion does not assure that the parameters of the variogram models fitted at contiguous anchor point will be consistent with each other. Thus, it needs to be complemented with criterions that enforce smoothly changing variogram parameter values.

Consistency between variogram models fitted at contiguous anchor points

If a wide enough kernel bandwidth is used to obtain the distance weights, the local experimental variograms change smoothly from one anchor point to another; therefore, the models fitted on them should also vary smoothly. The iterative fitting algorithm includes several measures aimed to enforce the consistency between the models fitted at contiguous anchor points. These measures applied to the local variogram model parameters are fourfold: (1) use of spatially correlated random alterations, (2) periodic averaging, (3) control of the local coefficient of variation, and (4) identification and correction of locally anomalous values.

The use of spatially correlated random alterations intends to minimize the occurrence of very divergent alternate fits among neighbouring anchor points. For creating random alterations with some degree of spatial continuity, the original array of uncorrelated random alterations is locally averaged within a window predefined by the user. This is performed at each iteration during the optimization process.

Smoothly changing local variogram model parameters can be obtaining by averaging the fitted values within moving windows. In a first optimization stage, this averaging is performed periodically after a number of iterations. If the locally averaged parameters lead to a lower objective function, the local averages replace the previous parameter values.

At the end of the first optimization stage, the algorithm calculates the local standard deviations and means of the parameter values within moving windows. In the second stage of optimization, the algorithm uses the local coefficients of variation obtained from these statistics as limits to the variability allowed in the selection of local parameters. If a local parameter value leads to a higher local coefficient of variability, this value is discarded, even if it leads to a smaller mean square error between the local experimental variogram and the local model.

The algorithm also identifies and replaces only the locally very high or very low parameters by the averages of the parameters fitted at neighbouring anchor point locations. The identification of these locally anomalous values is performed using a simple outlier detection criterion: the Q test for small datasets (Wellmer

1998, pp.60-61). At each neighbourhood V(**o**) containing $p_{V(\mathbf{o})}$ anchor points, the Q statistic for identifying an anomalously large local variogram model parameter b_β is obtained from:

$$\mathrm{Q}_1 = \frac{b_\beta(\mathbf{o}_1) - b_\beta(\mathbf{o}_2)}{b_\beta(\mathbf{o}_1) - b_\beta(\mathbf{o}_p)} \tag{5}$$

Where $b_\beta(\mathbf{o}_1)$ is the highest parameter value in the neighbourhood, $b_\beta(\mathbf{o}_2)$ is the second highest parameter value and $b_\beta(\mathbf{o}_1) - b_\beta(\mathbf{o}_p)$ is the local range defined by the highest and lowest parameter values in the neighbourhood. A Q statistic for identifying anomalously short local variogram model parameters is obtained from:

$$\mathrm{Q}_2 = \frac{b_\beta(\mathbf{o}_{p-1}) - b_\beta(\mathbf{o}_p)}{b_\beta(\mathbf{o}_1) - b_\beta(\mathbf{o}_p)} \tag{6}$$

With $b_\beta(\mathbf{o}_{p-1})$ as the second lowest local parameter value. . If $b_\beta(\mathbf{o}_1) = b_\beta(\mathbf{o}_p)$ it means that the local parameter values are the same for all anchor points in the neighbourhood; therefore, no outlier detection procedure is needed. Otherwise, if the Q_1 or Q_2 statistic exceeds a predefined threshold, the maximum value is considered as an outlier. Dean and Dixon (1951) tabulated the values of this threshold in relation to the number of observations. For the sake of computational simplicity and versatility the next curve provides a close fit to these thresholds:

$$\mathrm{Q}' \simeq 1.9622[p_{V(\mathbf{o})}]^{-0.687} \tag{7}$$

Figure 2 shows the fitting of the tabulated Q' values by the curve defined by this expression. Thus, if $\mathrm{Q} > \mathrm{Q}'$, the parameter value fitted at the anchor point **o** is replaced by the local average of the parameter values fitted at surrounding anchor points. Figure 2shows the tabulated and fitted values.

3. Description of the Algorithm

After reading and storing the experimental location-dependent variogram points and the corresponding sum of weights at different directions and for multiple anchor points the local variogram fitting algorithm proceeds as follows:

1. The global variogram model parameters are used as initial values in the minimization of the objective function (4).
2. In the first stage of the optimization process different combinations of azimuth and dip angles are sequentially chosen. For each combination, the other parameters are altered by arrays of spatially correlated random numbers. Only those alterations that lead to a minimization of the objective function are retained.
3. After 500 iterations, the variogram parameters are replaced by the local averages if they minimize the objective function. Another combination of angles is chosen. Points 2 and 3 are repeated until all azimuth and dip combinations are tested.
4. The local parameter sets that yield the minimum values of the objective function at the multiple anchor points are retained and used as initial values in the second stage of optimization. The local coefficients of variation of each parameter are calculated and kept for the second stage.
5. In the second stage of optimization the local nugget effect values remain unchanged from the previous stage. The remaining parameters are iteratively modified by the addition of spatially correlated random alterations. If an alteration results in a local coefficient of variation higher than the obtained at the end of the first stage, the alteration is rejected. After each of the iterations the locally anomalous parameter values are identified and replaced by local averages.
6. After ten thousand iterations the resulting variograms model parameters are written in an output file and the corresponding graphs generated.

4. Implementation

The proposed algorithm is implemented in the FORTRAN program `globfit`, which was developed from the `varfit` program (Larrondo, Neufeld, & Deutsch, 2003). As for the original `varfit`, the parameter file for `globfit` is divided in several sections.

The main section (see Figure 3) contains information about the number of directional variograms to fit, the number of structures, the weighting of the experimental points, the penalty function factors and the output files. The second section (see Figure 4) contains the specifications of the file with the output of the experimental local measures of correlations. This file is produced by the program `gamvlocal` (Machuca-Mory & Deutsch 2008a). This section also allows specifying a file containing the Hermite coefficients needed for performing the local back-transformation of the experimental variogram points obtained from locally or globally Gaussian transformed values (Guibal 1987; Vann & Sans 1995). If this file is provided, variogram fitting is performed on the backtransformed experimental variogram points.

The third section (see Figure 5) contains the specification of the global stationary variogram model. The stationary parameters will be used as initial values for the optimization process. The fourth section (see Figure 6) contains the specifications of the anchor points arrangement and the definition of the search window for neighbouring anchor points. The section of advanced parameters (see Figure 7) specify the parameters that will be fixed, treated as reference values, or allowed to freely vary within a range. It also allows the specification of the file containing the prior anisotropy orientation angles.

5. Testing

A 1-D dataset is used for testing the proposed algorithm. This dataset corresponds to the silver assays of a hole drilled in a high sulfidation polymetalic deposit. Figure 8 presents this dataset along with its corresponding local mean and standard deviations. The location-dependent experimental variograms were calculated using a Gaussian kernel of 40m bandwidth at anchor points separated by 1m.

Figure 9 shows the local nugget effect and the local vertical range fitted sequentially, but independently, with and without constraining the local nugget effect values. If the fitting of local variogram parameters is unconstrained, these can take extremely low or high values which may be unjustifiable in relation to the geological knowledge. Thus, as it is observed in Figure 9, the unconstrained fitting yields to very high local nugget effect values, and very short range values. Abrupt variations of these parameters are also observable in the unconstrained sequential fitting of location-dependent experimental variograms. If the local parameters are penalized outside a given range, 0.0 to 0.4 for the nugget effect and 10 to 200 for the variogram range in this case, the occurrence of extreme values is avoided. However, abrupt changes and locally anomalous values within the intervals defined by the user may still occur.

Figure 10 shows the resulting local variogram model parameters obtained using the `globfit` program with penalty factors from 0 to 0.1. Abrupt changes in the local variogram parameters still occur for low penalty values, but the isolate locally anomalous parameter values are eliminated. In this case, with a penalty factor above 0.1 the local nugget effect and variogram range seldom exceed the specified allowable ranges. Lower penalty factors can be selected in order to allow some flexibility in the fitting of the experimental location-dependent variograms.

Figure 11 shows the final values of the objective function obtained by the independent sequential automatic fitting and by `globfit`. In general, the final objective function values are lower when `globfit` is used. Note the areas were the final objective function values of the independent sequential fitting are much higher than those obtained by `globfit` correspond to areas where the fitted parameter values diverge abruptly from the local tendencies.

Figure 11 shows the final values obtained in the minimization of the objective function. This is the addition of the mean square error between the experimental points and the final local models plus the penalties to parameter values exceeding the predefined limits. Thus a lower final objective function value does not imply necessarily a closer fit to the local experimental variograms points

6. Conclusions

Fitting multiple local variogram models at multiple anchor point locations is only feasible with the help of an automatic fitting algorithm. Independent automatic fitting of location-dependent experimental variogram models can yield to abrupt variations in the fitted local parameters. These variations are usually at odds with the usually smooth change of these local 2-point statistics between closely located anchor points. They tend to occur when the location-dependent experimental variogram points are highly discontinuous from one lag to another. `globfit` is able to minimize the occurrence of abrupt changes in the variogram model parameters and it is also able to identify and correct isolated very high or very low parameter values. This is done mainly by controlling the coefficient of variation of the local variogram parameters and by applying a procedure for the detection and averaging of local outliers. `globfit` also allows the user to control the range of values that local variogram model parameters can take. Additionally, `globfit` allows the incorporation of local orientations for guiding the fitting of anisotropy angles and also allows the fitting of locally backtransformed Gaussian variograms.

The testing of this program has been limited so far to 1-D and simple 2-D datasets. More testing is required for 2-D and 3-D datasets for cleaning possible programming bugs and assessing all the capabilities this new program offers.

References

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Figures

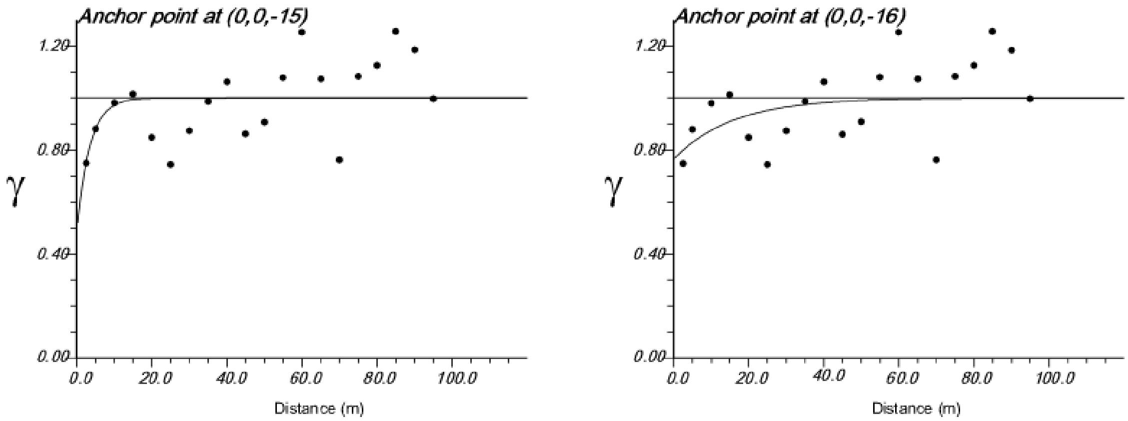

Figure 1: Different local variogram models (continuous curves) fitted at adjacent anchor points with practically similar local experimental variograms (dots).

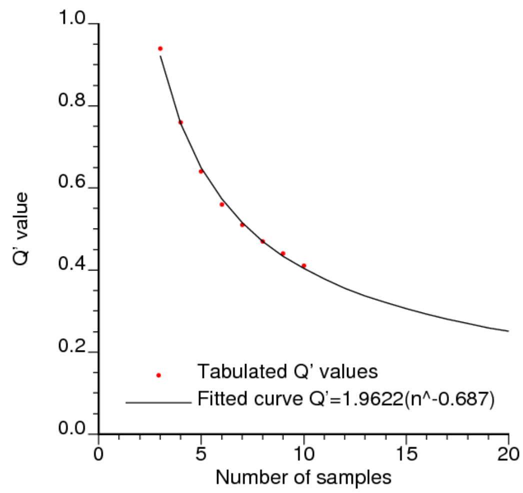

Figure 2: Tabulated Q' values and approximation by a power function

```
                  Parameters for GLOBFIT
                  **********************

START OF MAIN PARAMETERS:
3                          - number of variograms
1                          - number of nested structures
1                          - constant angle between structures
1                          - inverse distance weighting (0=no, 1=yes)
0                          - pairs  weighting (0=no, 1=yes)
0                          - variogram variance weighting (0=no, 1=yes)
10                         - minimum number of pairs to use
0.05                       - penalty constant for extreme parameter values
./graphs/corfit            - file for PostScript output
corrfit.var                - file for variogram model
corrfit.sum                - file for summary file
Local rho with fitting penalty = 0.05 iw  -project title
```

Figure 3: Main parameters for `globfit` program.

```
START OF EXPERIMENTAL VARIOGRAMS SPECIFICATION:
0                          - Fitting Z variograms from Y values? (no=0, yes=1)
herpol.dat                 - file with Hermite coefficients
30 1                       - number of hermite polynomials and column for phi(0)
1-rDDH75_lns_40.out        - variogram #1 file
   1                       - variogram number in file
1-rDDH75_lns_40.out        - variogram #1 file
   2                       - variogram number in file
1-rDDH75_lns_40.out        - variogram #1 file
   3                       - variogram number in file
```

Figure 4: Specification of the files containing the local experimental variograms and the local Hermite. Coefficients

```
START OF GLOBAL VARIOGRAM MODEL SPECIFICATION:
0.123   0.439              - nugget effect, exp
2  0.877  0.0  0.0  0.0    - it,cc,ang1,ang2,ang3
          7.6  7.6  7.6    - a_hmax, a_hmin, a_vert
```

Figure 5: Parameters of the globally stationary variogram model.

```
START OF ANCHOR POINTS DEFINITION
400                        - number of anchor points
4                          - maximum number of anchor points for parameter comparison
20.0  20.0  20.0           - maximum search radii
 0.0   0.0   0.0           - angles for search ellipsoid
```

Figure 6: Definition of the anchor points arrangement and search window.

```
START OF ADVANCED OPTIONS:
0    0    0          - zonal Anis: Hmax, Hmin, Vert (0=no, 1=yes)
0    0    0          - cyclicity:  Hmax, Hmin, Vert (0=no, 1=yes)
0  1.0  1.0          - Variable initial Sill (0= no, 1 = yes), lower and upper tolerance
0  0   0.4           - Variable initial nugget effect (0=no, 1=yes), lower and upper limits
1                    - number of structure types to fix
1  2                 - structure number and structure type (6=stable variogram model)
0.5  2.0             - Lower and upper limits for stable variogram exponent
1                    - number of Hmax ranges to control/fix
1  10  180           - structure number, lower and upper limits
1                    - number of Hmin ranges to fix
1  5   100           - structure number, lower and upper limits
1                    - number of Vert ranges to fix
1  2.5  80           - structure number, lower and upper limits
ackt3d_ang.out       - file with prior local anisotropic angles
1 2 3                - columns for local ang1, ang2 and ang3
1                    - number of azimuth angles to control/fix
1   0.0  180.0       - structure number, lower and upper limits
1                    - number of dip angles to control/fix
1   0.0  90.0        - structure number, lower and upper limits
1                    - number of plunge angles to control/fix
1  -90.0  0.0        - structure number, lower and upper limits
0                    - number of variogram preferences
1                    - number of Hmax/Vert anis. to control/fix
1   0.5    1.0       - structure number, lower and upper limits
1                    - number of Hmin/Hmax anis. to control/fix
1   0.5   1.0        - structure number, lower and upper limits
```

Figure 7: Advanced parameters for `globfit`.

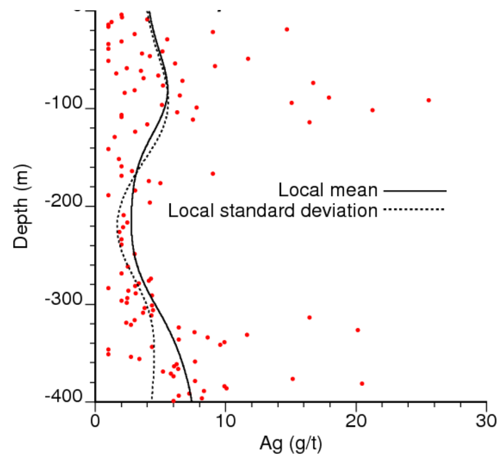

Figure 8: 1-D testing dataset with its corresponding local means and local standard deviations.

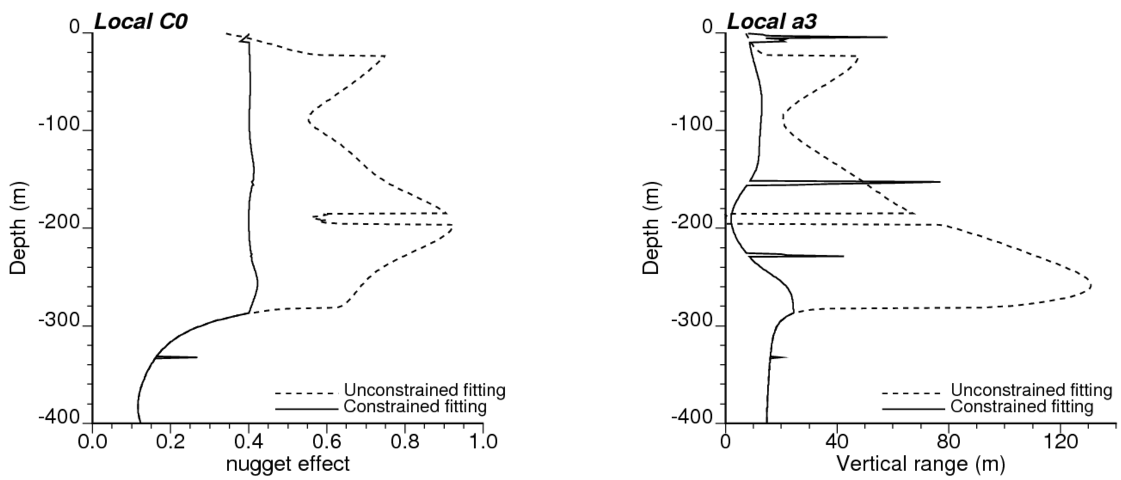

Figure 9: Local nugget effect (left) and variogram range (right) obtained by sequential independent automatic fitting of local experimental variograms with penalization of nugget effect values above 0.4 (continuous line) and without it (dashed line).

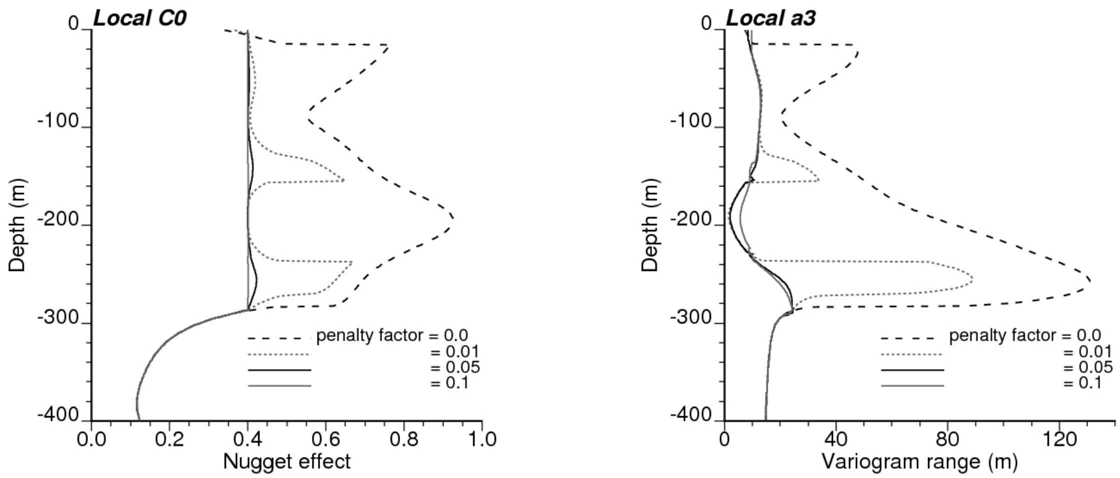

Figure 10: Local nugget effect (left) and local variogram ranges (right) obtained with the program `globfit` using different penalty factors for values exceeding 0.4, for the nugget effect, and outside the interval of 10 to 200m, for the variogram range.

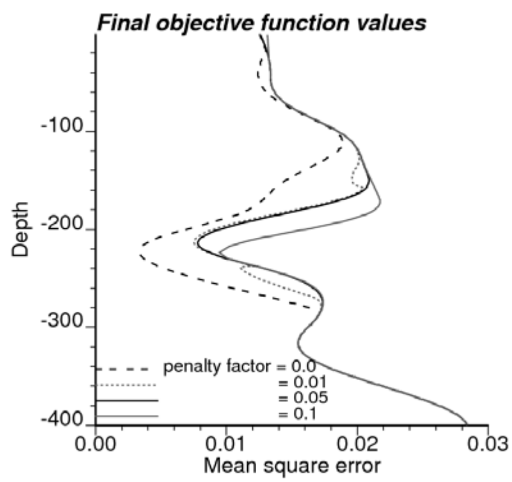

Figure 11: Minimum objective function values obtained by sequential independent automatic fitting of local experimental variograms and by `globfit`.