Validation and Confirmation of Non-Stationary Models with the Ventersdorp Reef Data

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Validation criteria for non-stationary parameters and the models generated using them within a locally-stationary framework are presented and discussed. A smooth and unbiased adaptation of the local parameters to the variations informed by data values is important. The criteria for simulated models are the reproduction of the input data and the input models of spatial continuity. These validity criteria for parameters and numerical models are illustrated with the help of a sparse data set that mimics samples taken from drillholes interception the Ventersdrop Contact Reef. A denser data set is used for confirming the initial local models of spatial continuity and the realizations generated using them. Local data scarcity and short scale variations of the spatial distribution appear to be the main difficulties in the confirmation of the initial local variogram models. Simulated models satisfy minimum validity criteria, such as the reproduction of the global histogram and the local spatial continuity informed by location-dependent variogram models. The confirmation of the distributions of uncertainty indicate that the realizations produced by locally stationary indicator simulation may yield to a fairer uncertainty than those produced by standard indicator simulation.

Introduction

Distance weighted distributions and statistics are aimed to reflect non-stationary aspects of the spatial distribution of a geological attribute (Brundson, Fotheringham, & Charlton, 2002; Lloyd, 2007; Machuca-Mory & Deutsch, 2008b). A locally anchored distance weighting function modifies the global distribution and statistics by assigning higher weights to closer samples (Machuca-Mory & Deutsch, 2008a). The resulting local statistics and the parameters fitted on them are used in spatial prediction under the assumption of local stationarity (Machuca-Mory & Deutsch, 2008c). The numerical models produced by locally stationary techniques, and their input local statistics and parameters, required a minimum of validation criteria. Most of these criteria are akin to the used on the models generated by traditional methods. However, the use of locally changing statistics and parameters demand additional criteria and pose new challenges. This paper presents some validation criteria for non-stationary models and discuses their particular issues. The Ventersdorp Reef dataset is used for illustrating several of these validation criteria. This dataset is also used for the confirmation of the locally stationary models.

The terms validation and confirmation are used in concordance to the discussion by Oreskes et al. (1994). In this sense, and in the context of this paper, validation is referred to the consistency of the locally stationary methods in relation to initial data and input parameters. Confirmation of the models is performed by assessing the match between model predictions and additional data.

A brief description of the Ventersdorp Contact Reef Data set and the subsets used for validation and confirmation is presented first. For the sake of brevity only categorical data corresponding to the most important facies is used in this work. The criteria for choosing the distance function parameters are discussed next. The location-dependent variogram models fitted with the initial data set is compared with the local variograms modeled on the much denser confirmation dataset. Locally Stationary Sequential Indicator Simulation (LSSIS) is performed using the initial dataset and the location-dependent parameters obtained from it (Machuca-Mory & Deutsch, 2009). The simulated models are validated in relation these data and parameters. The accuracy and precision of the LSSIS model are checked using the confirmation dataset and the results are compared with those obtained from models generated using traditional Sequential Indicator Simulation (SIS). A brief discussion of the main issues encountered is presented at the final part of the paper along with an outline for future work.

The Ventersdorp Contact Reef Data Set

The samples used in this paper are a small subset of a much denser channel sampling dataset, which was taken from the underground operations at the VCR. This goldfield is located at the northern fringes of the West Rand Group in the Witwatersrand Basin. This is formed by mineralized conglomerates arranged in well defined channels (Moon, Whateley, & Evans, 2007). It is known that sedimentological factors seem to control the spatial distribution of gold grades in the conglomerates. However, for this case study, the geological information available for this data set is limited to the numerical coding of four different facies. The geological description of these facies was not provided whatsoever.

Figure 1a presents a map of the complete dataset showing the locations of 161,179 channel samples coloured by facies codes. The complete data set was sampled in a 200m x 200m quasi regular grid simulating drillhole intercepts in the reef. This grid spacing is within the typical range for exploration drilling meshes of the deep gold reefs in the Witwatersrand (du Pisani & Vogt, 2004) . Only the intercepts located in Facies 1 and 2, which are the most important, are considered for the initial dataset. These correspond to 181 simulated drillholes. This number is comparable to the number of holes drilled at other properties in neighbouring goldfields (Rance, et al., 2006). Around each drillhole, the closer four samples within a 15m radius were collected. This was done in order to simulate the wedge deflections commonly drilled in order to increase the number of reef intercepts at a minimum number of additional drilling (Magri, 1987). Figure 1b shows the locations of the 782 channel samples selected as simulated drillhole and deflections intercepts within the boundaries of Facies 1 and 2. The confirmation dataset was generated by randomly picking one tenth of the samples in the complete dataset. This amounts to 14380 samples located in Facies 1 and 2. Table 1 summarizes the declustered indicator statistics of Facies 1 in the initial, the confirmation and the complete datasets.

Table 1: indicator statistics for Facies 1

Dataset :	Initial	Confirmation	Complete
Number :	782	14380	143445
Proportion :	0.236	0.240	0.240
Variance :	0.180	0.182	0.182

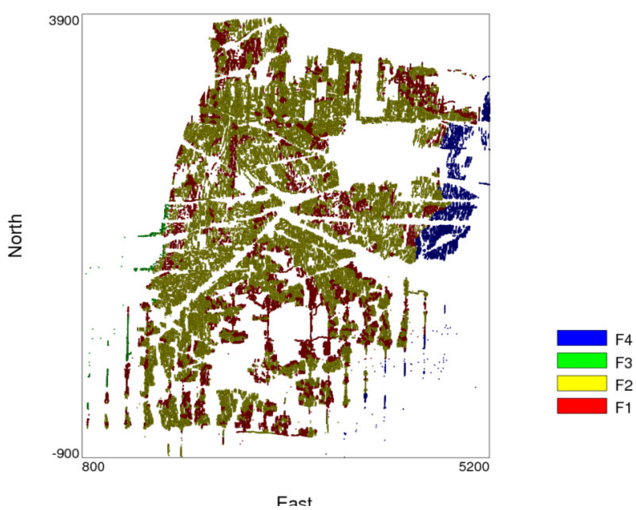

Figure 1a: Complete VCR channel sampling data set coloured according the Facies.

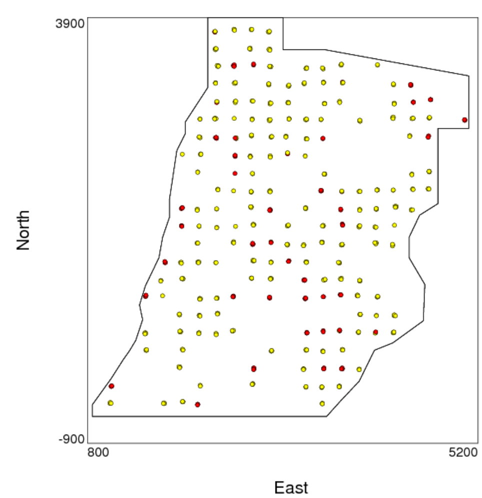

Figure 1b: Locations of simulated drillhole and deflections

Selection of weighting function parameters for location-dependent statistics

The distance weights for inference of location-dependent distributions and statistics should be such that allow a smooth adaptation of the local parameters to the variations informed by data. Smoothness is an important criterion for several reasons: it is coherent with the lack of information at higher resolutions, it filters variations caused by local outliers, it assures the stability of the local models, and it permits enough flexibility in the estimation of the local distributions during spatial prediction. Contrarily, highly variable location-dependent statistics are difficult to justify, particularly when data is sparse, for they may be caused by artifacts or by the influence of values that are not representative of the local distributions. The models fitted on highly variable local measures of spatial continuity are usually unreliable.

In spatial prediction with a trend model of the local mean, the deterministic component of the Random Function is assimilated to the trend, while the probabilistic component is left to the residuals. If the trend overfits the data, the uncertainty of the numerical models is artificially diminished. The same idea can be extended to the all local statistics required in locally stationary techniques. Finding a reasonable trade-off between local adaptation and smoothness is in great extend a subjective exercise. Smoothness is in the eye of the beholder; a fair model of location-dependent statistics is normally chosen by visually comparing maps obtained using different parameters for the distance weighting function. A rule of thumb is to choose the model that shows less structures circumscribed at very few sample locations, but shows tendencies informed by numerous samples.

A Gaussian kernel (GK) is a preferred distance weighting function because its simplicity and its ability to yield smooth estimates. The smoothness of locally weighted statistics is controlled by the bandwidth and background parameters of the GK (Machuca-Mory & Deutsch, 2008a). Figure 2 presents three local mean models obtained using GK functions with 200m, 300m and 400m bandwidth and a background of 0.01. The 200m bandwidth model presents structures controlled by few sample locations, while the 400m bandwidth model appears too smooth. The 300m bandwidth model is a reasonable intermediate election. The same observations can be derived from the models of local variance in Figure 3.

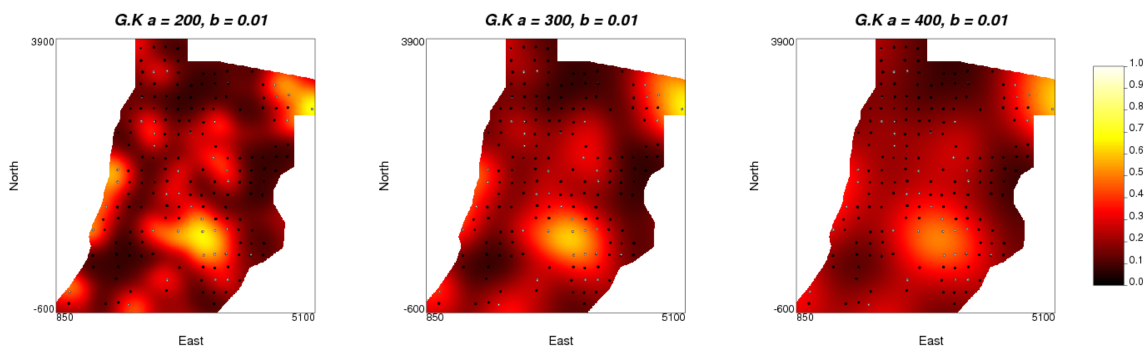

Figure 2: Local proportion models obtained using Gaussian Kernel functions with different bandwidths

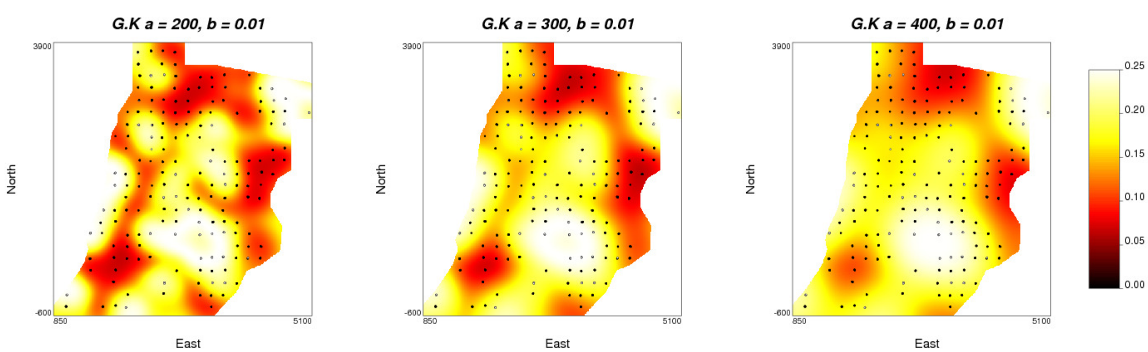

Figure 3: Local variance models obtained using Gaussian Kernel functions with different bandwidths

Despite being mostly subjective, the election of the weighting function parameters can be backed by numerical criteria such as the ratio trend/data variance and the coefficient of correlation between trend and data values. If the local mean model is smooth, its variance represents a limited fraction of the data variance. It has been suggested, as a rule of thumb, that this fraction should not exceed 50% (McLennan, 2007). This criterion is expressed as:

$$\sigma^2_{m(\mathbf{u})} \Big/ \sigma^2_Z < 0.5 \tag{1}$$

If the local mean model adapts to local changes, the coefficient of correlation between trend and data values should be at least moderately positive. This criterion is expressed as:

$$\max\left[\frac{C_{m(\mathbf{u})Z}}{\sigma_{m(\mathbf{u})}\sigma_Z}\right] \tag{2}$$

Figure 4, left, shows the variance ratio for mean trend models obtained with different parameters of the GK function. Figure 4, right, shows the coefficient of correlation between these trend models and the initial dataset indicator values. A GK function with 300m bandwidth and background value of 0.01 produces a trend model with small variance and reasonably high coefficient of correlation.

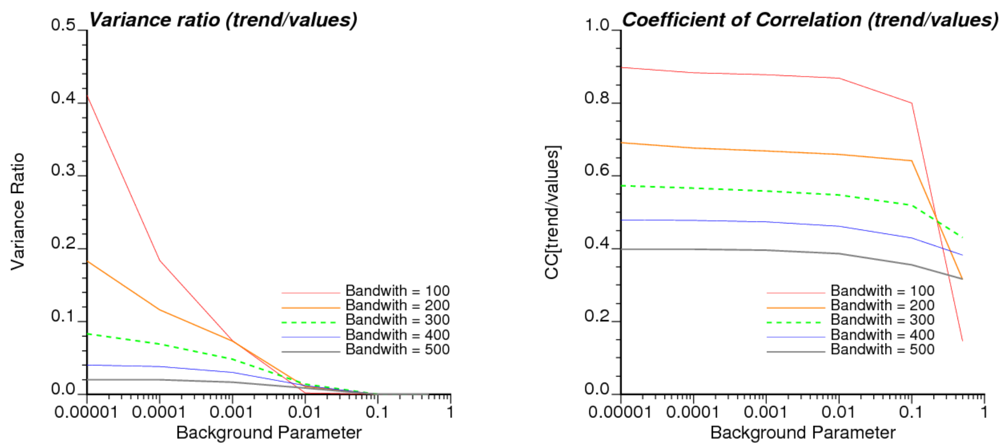

Figure 4: Ratios trend / data variances (left) and coefficient of the correlation between the trend and data values (right) for the local proportion models using different Gaussian Kernel parameters.

An important numerical check on the local mean model is the match of the global declustered data mean by average of the local trend values. A mismatch between these two means would suggest the presence of bias either in the global stationary mean or in the local mean model. The first situation may be caused by a deficient declustering method or parameters, while in the second case the bias may be introduced by the distance function. The average of local proportions of Facies 1 is 0.235, which is reasonably close with the average global proportion shown in Table 1.

For the Additional considerations for choosing the distance weighting function parameters are the data density and the scale of modelling. If sampling is dense, it is possible to use smaller bandwidths in order to resolve the local statistics at a relatively small scale. In this sense, another advantage of the kernel distance methods is that the bandwidth can be selected in relation to the sampling separation and the scale of modelling. Moreover, if the scale of the non-stationary features can be obtained from secondary information or abundant data, it can also be used for tuning up the distance function parameters.

Ideally, all the location-dependent statistics should be inferred at every location in the model using the chosen distance weighting function. For 1-point statistics this can be accomplished straightforwardly. However, for 2-point statistics, this can be very demanding in computer resources. Additionally, checking the local statistics and the models fitted on them would be tedious if it is done at every location. Alternatively, the 1-point and 2-point local statistics obtained for a limited number of anchor points can be interpolated for all other locations. The spacing of the anchor points must be such that the interpolated statistics and parameters closely match those that would be inferred with no interpolation at every location. Normally this is achieved when anchor point separation is smaller than the GK bandwidth. For this case, an anchor point grid of 200m x 200m was selected. Figure 5 shows the 312 anchor points within the modelling boundary along the sample locations.

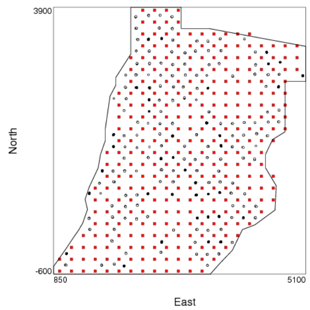

Figure 5: Locations of anchor points in relation to samples.

Validation and confirmation of the location-dependent correlograms

The experimental location-dependent indicator correlograms (Machuca-Mory & Deutsch, 2009) were calculated for 6 directions at each anchor point of Figure 5 using the weights obtained with a GK function of 300m bandwidth and background value of 0.01. The 312 sets of directional local correlograms were fitted automatically using a single exponential variogram structure. As for local means and variances, the fitted variogram parameters are expected to vary smoothly for the reasons explained before. Abrupt changes from one anchor point to another were identified and substituted by alternative fits. 13% of the original local variogram models were substituted by models fitted giving more weight to the closest experimental points and to those calculated with higher number of nearby pairs. Figure 6 shows maps of the interpolated parameters of the local variogram models.

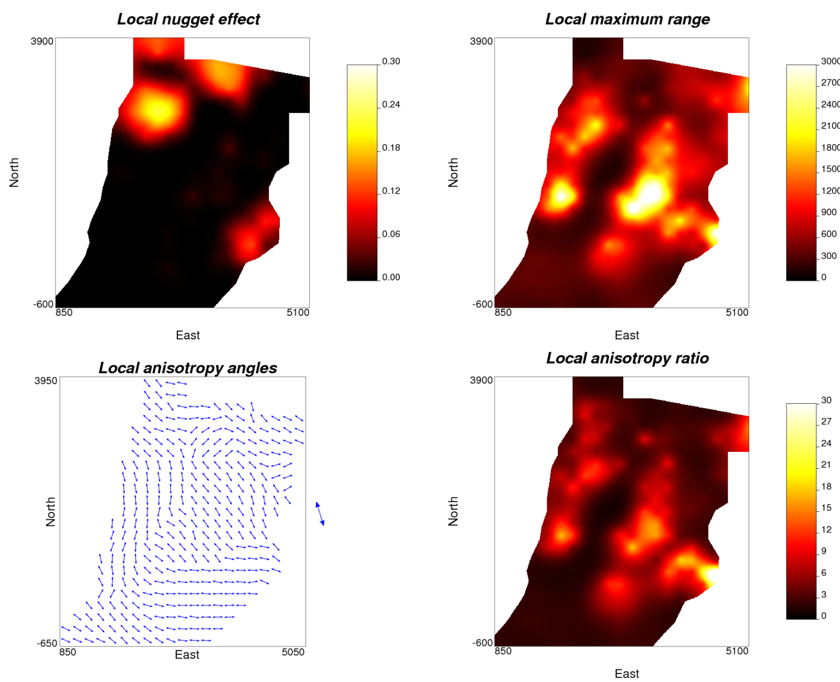

Figure 6: Interpolated maps showing the local parameters of the variogram models fitted on the location-dependent experimental correlograms of the initial dataset.

Besides smoothness, the local variogram parameters can be validated by their correspondence with the geological knowledge basis, if available, and, if data is dense enough, with the spatial features observed on it. Unfortunately, no geological information on the geometry of facies is available, and the initial data set is so sparse at some areas for drawing reliable visual interpretations by hand.

The confirmation dataset was divided in subgroups within circular windows of 400m radius centred at the anchor points. Traditional experimental correlograms were calculated only for subgroups with more than 100 samples. The corresponding models fitted also automatically. Figure 7 shows the parameters of the fitted local variogram models. They appear more variable than the local parameters for the initial dataset. The abundance of closely spaced data provides better information on the short scale variability. This translates in higher local nugget effect and shorter local variogram ranges at most locations. Figure 8 shows maps of the magnitude of the differences between the parameters of local variogram models fitted on the initial dataset and those corresponding to the confirmation dataset. Discrepancies between local parameters, particularly for the local anisotropy orientation, are generally higher in areas with low sample density, or where the scale of anisotropic features is smaller than the initial dataset spacing.

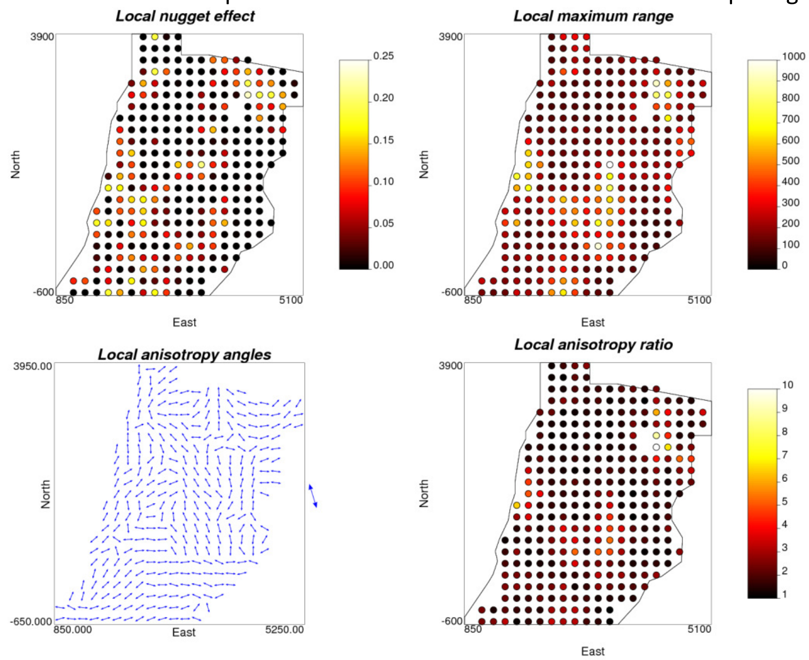

Figure 7: Local parameters of the variogram models fitted on the experimental correlograms calculated using the confirmation data within windows of 400m radius centred at the anchor points.

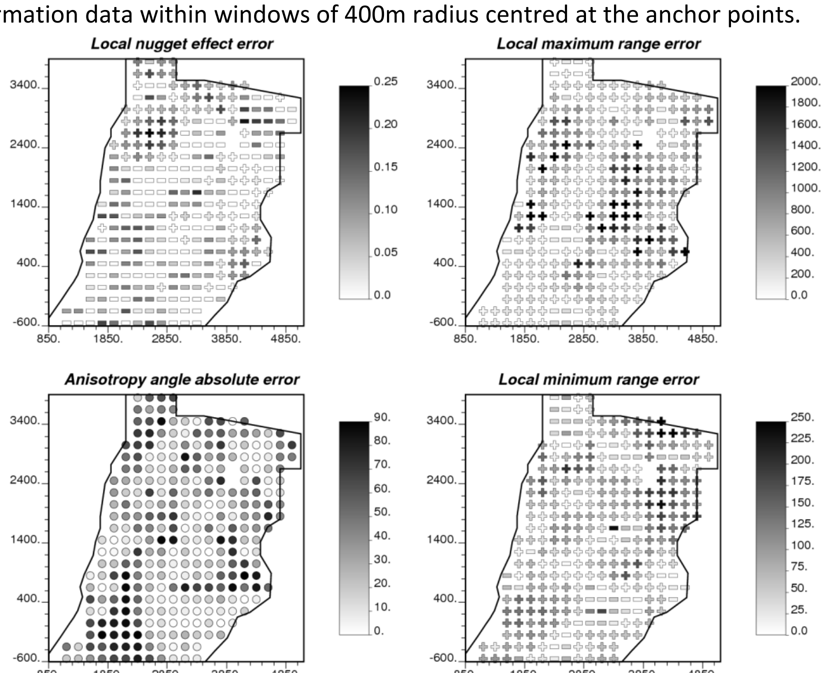

Figure 8: Difference between the local variogram parameters of the initial dataset and the corresponding to the confirmation dataset. A plus sign indicates that the local parameter is greater for the initial models than for the confirmation models. A minus sign indicates the contrary.

Validation and confirmation of locally stationary numerical models

The minimum validity criteria for realizations generated by stationary geostatistical simulation methods is the reproduction of data values at each sampled location, and also, within acceptable ergodic fluctuations, of the data cdf and of the input variogram model (Leuangthong, McLennan, & Deutsch, 2004). Similar criteria can be applied for locally stationary realizations. If data values are assigned to the closer node, data reproduction is normally satisfied unless particular circumstances, such as the presence of multiple samples within a cell, or if the samples are flagged as outliers, or they fall outside the grid model.

Although the locally stationary methods work with local distributiona, the reproduction of the global cdf is still the aim. A considerable divergence between the realizations global cdfs and the global data cdf may indicate a bias introduced by the location-dependent distributions. These local distributions, instead, do not need to be reproduced, since they are used only as prior models of local uncertainty, which are updated by simple kriging using the surrounding data and the location-dependent variogram models.

Contrarily to the data histogram, the local variogram models, rather than the global, must be reproduced. However, due to their locally stationary nature, the reproduction of these models can only be validated for short distances. Checking the local variogram reproduction may be tedious, since multiple experimental variograms must be calculated at different locations for all realizations. Simple checks as the visual verification of the reproduction of the anisotropic features in the realizations may be performed.

Beyond these minimum model checks, validation techniques that can be applied to locally stationary models include cross-validation, the jackknife and the distributions uncertainty check (Deutsch, 2002). Cross validation of locally stationary models can be performed in the traditional way, this is masking only sample or an entire drillhole and re-estimating at these locations with the surrounding data and previously defined local models, or by inferring the local statistics without the masked data and estimating with the resulting local parameters. In the standard cross validation of locally stationary models, some of the information provided by the masked data is implicit in the local prior distributions and statistics inferred with the complete dataset. The second variant of cross-validation is more complete and stricter. This can be used to assess the stability of not only the estimation parameters but of the location-dependent statistics themselves.

The jackknife approach applied to the validation of locally stationary models consists in dividing the dataset in different non-overlapping subsets, inferring the location-dependent distributions and statistics for each of these subsets, and re-estimating each subset with the values and local parameters of a non-overlapping subset. The jackknife is feasible only for large datasets, since the diminished number of samples in each subset may difficult the inference of local statistics. If data is abundant enough, this validation technique can be used for assessing the robustness of the location-dependent statistics and the parameters of models fitted on them prior to the estimation. This approach is already demanding in computational and professional effort when applied to stationary models, it can be much more demanding when used in the validation of locally stationary models. For both, cross validation and jackknife, the distribution of the estimation errors should be symmetric, with a zero mean and a minimum variance, and the errors should be independent from each other.

Accuracy plots (Deutsch, 1996) are used for checking the distributions of uncertainty of the numerical models. Given a probability interval, p, the distribution of uncertainty is said to be accurate and precise if the proportion of true values that fall within this interval defined in the model distribution is also p. If this proportion is greater than p, it would indicate an excessive uncertainty in the model, whereas if it is smaller, it would indicate a too narrow uncertainty. The true values and local distributions of uncertainty needed for building the accuracy plot can be obtained from the results of cross validation and jackknife. Accuracy plots can also be used for confirming the uncertainty models when additional data is available

Fifty LSSIS realizations where generated using the local facies proportions and indicator variogram parameters corresponding to the initial dataset. Figure 9 presents an example LSSIS realization along with an equivalent traditional SIS realization. The effect of using locally changing variograms in locally stationary model is clear. The reproduction of the initial facies proportions by the realizations is acceptable. The average proportion for Facies 1in the 50 realizations is 0.23 (see Figure 10, left). The

reproduction of the local anisotropy informed by the local variogram models is checked by visual comparison with the e-type estimates map (see Figure 10, right).
The confirmation data set was used for confirming the distributions of uncertainty given by the multiple realizations. Accuracy is difficult to achieve with the sparse initial dataset. However LSSIS realizations show a fairer uncertainty width when compared with standard sequential indicator simulation.

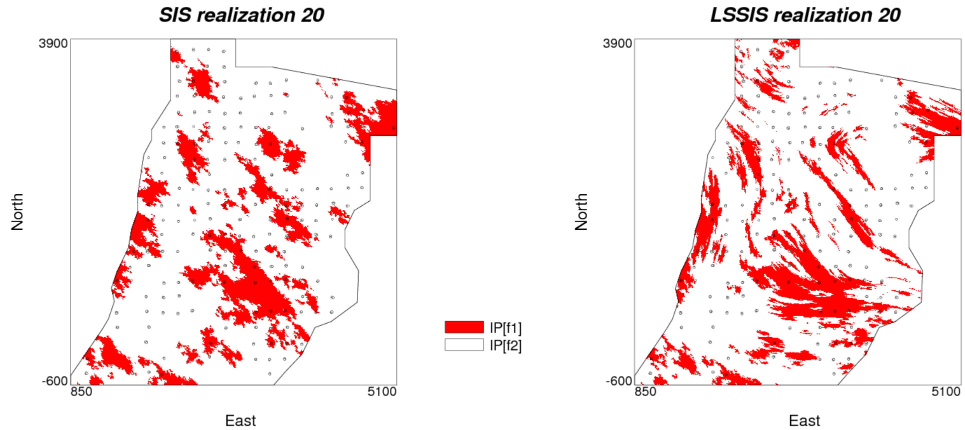

Figure 9: A traditional SIS realization along with an equivalent LSSIS realization.

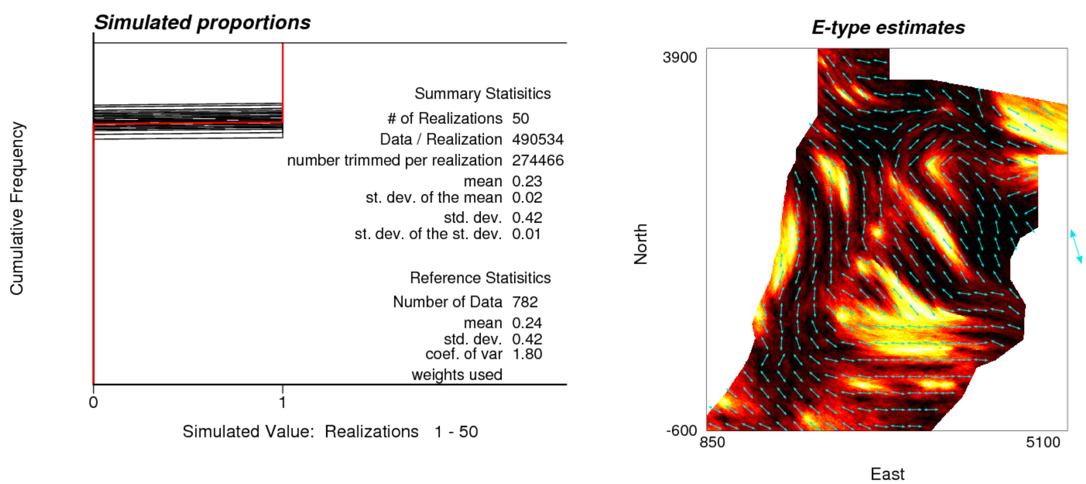

Figure 10: Reproduction of the global facies proportions by LSSIS realizations (left). Reproduction of the anisotropy orientation of local variogram models reflected on LSSIS e-type estimated.

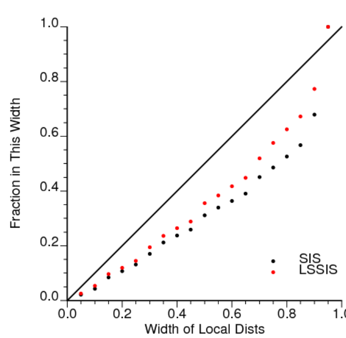

Figure 11: Accuracy plots for SIS and LSSIS realizations obtained by comparing the distributions of uncertainty in the simulated models with the distribution of the confirmation dataset.

Discussion and Future Work

Most of the validation criteria for locally stationary parameters and the numerical models generated using them is borrowed from the criteria used for stationary models. However new issues appear under the locally stationary framework. In absence of a geological knowledge basis or of secondary correlated information that could be used for guiding and validating the local statistics inference, the variation of location dependent statistics is extracted only from the available primary data. In this context, smoothness of the local statistics is required, since lack of it would indicate the local preponderance of single or very few samples or may reflect artifacts caused by the local inference methodology. The variation of local statistics should respond to tendencies in the data at a scale larger than the sample separation. Inference of local statistics becomes more difficult when data is scarce, since individual samples, rather than local groups, acquire relevance. If it is the case, the use of traditional techniques is preferred. Contrarily, if data is abundant enough, the jackknife technique can be used for testing the robustness of location-dependent statistics.

This fitting of local variogram models is still an important issue, for it may also introduce locally anomalous parameter values. When this occurs alternative model fits using different weighting schemas for the experimental variogram points are considered. A more robust fitting algorithm for location-dependent variograms that minimize the occurrence of abrupt changes in the local parameters is required.

Normally, the location-dependent statistics and parameters inferred from sparse data will be satisfactorily confirmed at some location, while the will turn wrong in others when compared with the equivalent statistics and parameters inferred from denser data. The higher discrepancies are observed in areas where data is scarce or where changes in the spatial continuity of the attribute occur at a shorter scale than the original sampling separation.

Locally stationary simulation techniques fulfill satisfactorily the minimum validity checks for geostatistical realization. The global histogram is reproduced, as well as the local directions of spatial continuity informed by the location-dependent variogram models. Checking the reproduction of other characteristics of local variograms, such as the ranges and the nugget effect, requires the development of an algorithm that would abbreviate the tedious task of recalculating the local experimental variograms at different locations and for all realizations. Confirmation of the distributions of uncertainty by denser data indicates that, although it is difficult to obtain acceptable accuracy with very sparse data, the uncertainty of LSSIS realizations may be fairer than the obtained by traditional SIS.

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