Transformation of Residuals to Avoid Artifacts in Geostatistical Modelling with a Trend

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Abstract

Trend modelling is an important part of natural resource characterization. A common approach to account for a variable with a trend is to decompose it into a relatively smoothly varying trend and a more variable residual component. Then, the residuals are stochastically modelled independent of the trend. This decomposition can result in values outside the plausible range of variability, such as grades below zero or ratios that exceed 1.0.

We transform the residuals conditional to the trend component to explicitly remove these complex features prior to geostatistical modelling. Back transformation of the modelled residual values allows the complex relations to be reproduced. Mining and petroleum related applications show the robustness of the proposed transformation.

Introduction

Geostatistics is increasingly popular for natural resource characterization. The tools provide the ability to construct geologically realistic models. These tools, however, rely on some basic assumptions to permit inference of the spatial statistics at unsampled locations. Geostatistical models depend on a decision of stationarity that assumes invariance of the multivariate cumulative distributon function (cdf) over the domain, that is

$$F_{Z(\mathbf{u}_1),\ldots,Z(\mathbf{u}_N)}(z(\mathbf{u}_1),\ldots,z(\mathbf{u}_N)) \quad = \quad F_{Z(\mathbf{u}_1+\mathbf{h}),\ldots,Z(\mathbf{u}_N+\mathbf{h})}(z(\mathbf{u}_1+\mathbf{h}),\ldots,z(\mathbf{u}_N+\mathbf{h})), \forall \mathbf{h}$$

For practical purposes, second order stationarity is assumed explicitly for geostatistical inference, that is $E\{Z(\mathbf{u})\} = \mu$ and $Cov\{Z(\mathbf{u})\cdot Z(\mathbf{u}+\mathbf{h})\} = C(\mathbf{h}), \forall \mathbf{h}$ and $\mathbf{u} \in A$. Multivariate stationarity is implicit to the particular geostatistical implementation.

For most practical problems, spatial trends violate this assumption and the application of geostatistical methods is no longer straightforward. Real data often exhibit spatial trends in the first and/or second moment. For example, it is common to have regions of low and high grades within a mineral deposit. Further, the variability within these regions may change depending on the grades. Direct application of common geostatistical tools may inappropriately spread (or smear) spatial features across different areas; trend modelling becomes an integral component to the geostatistical work flow.

A further complication is the subjectivity of trend detection and modelling. There is no "objective" way to determine that there is a trend. The existence of a trend and how to model it is very much dependent on the practitioner. Trends depend on many factors, including the data available and the scale of observation. Although it is common for most trends to be modelled arbitrarily by a decomposition approach, the practitioner's experience with similar deposits/reservoirs may also affect the trend model.

This paper discusses some of the methods to detect and model a trend, but will focus primarily on the additive decomposition of the random variable into a mean and residual. Common problems associated to this decomposition will be addressed, and a transformation to handle these problems will be presented.

Detecting Trends

In some cases where the depositional environment is well understood, trends can be detected by geological knowledge of the site of interest. In most cases, however, the data are the source for trend detection. Large scale spatial features can be detected during several stages of data analysis and modelling. Sometimes a simple crossplot of the data against elevation may show a trend (Figure 1). To visualize trends, a moving window average of the data can be calculated to determine if local means and/or variances are indeed stationary. The size of these "windows" will depend on the number of data available. Also, if few data are available, then these windows may overlap so as to permit more reliable calculation of the local statistics [4, 6]. If there are notable changes in the local mean and variance within the domain, the practitioner may decide that there is a spatial trend.

Although the identification of a trend is subjective, it is widely accepted that the trend is essentially deterministic and should not have short scale variability. Any features that are not significantly larger than the data spacing should probably be left for stochastic modelling.

One further step is to examine the data for a proportional effect, that is, whether the local variance is dependent on the local mean. In general, a crossplot of the local mean and the local variance can show this phenomenon. In the presence of a proportional effect, the relation between the local mean and variance is often quadratic. Our proposal consists of transforming the residuals to be independent of the mean. This correction will often account for the proportional effect; however, some basic checks during model construction can be used to see if further steps are required.

Another stage of the modelling process where spatial trends may be evident is during variography. The experimental variogram may show a trend in any one or more of the principal directions. This is easily identified as the experimental variogram continues to increase above the variance of the random variable as the lag distance, $\mathbf{h}$, increases (Figure 2). This usually indicates that the practitioner should revisit their decision of stationarity and consider whether the domain should be subdivided or a trend considered.

Common Trend Modelling Approaches

The most common and straightforward approach is to separate the RV into two components - the trend and the residual:

$$Z(\mathbf{u}) = m(\mathbf{u}) + R(\mathbf{u}) \tag{1}$$

where Z is the original RV, m is the trend or mean component, R is the residual RV, and $\mathbf{u}$ denotes the location, commonly representative of Cartesian coordinates (x, y, z). This type

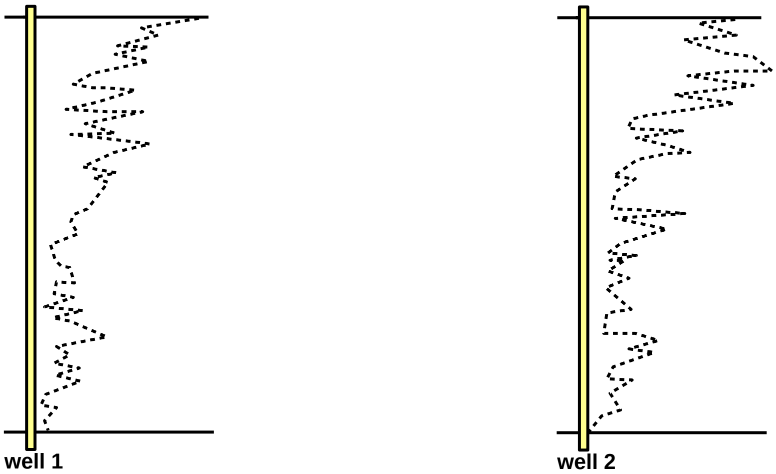

Figure 1: Example of vertical trend as indicated by two well logs. (Source: Deutsch, 2002)

of decomposition correspondingly leads to a decomposition of the total variability of the original RV:

$$\sigma_Z^2 = \sigma_m^2 + \sigma_R^2 + 2C(R, m) \tag{2}$$

where σ_Z^2 is the variance of the original RV, σ_R^2 is the variance of the residual RV, and $C(R, m)$ is the covariance between the residual and the mean components. This covariance can be either negative or positive; however, if this value is close to zero, fewer artifacts associated to the decomposition are expected [2].

The mean component is defined at all locations via a 3D trend model, while the residual values are only defined at data locations [2]. Geostatistical modelling is then only performed on the residuals that are considered to be stationary. Multiple realizations of the residuals are generated and added back to the single trend model to produce multiple realizations of the original RV.

The problem remains as to how the trend should be "modelled" so as to obtain a stationary residual random function (RF) for geostatistics. The idea is to obtain a model that accounts for large scale variability; small scale variability is accounted for in geostatistical modelling of the residuals. As a result, trend models are typically smooth models constructed through interpolation *and* extrapolation of the trend data. In areas of interpolation or within the range of the data, there may be no need for a trend model - the model values will be influenced and/or controlled by the data.

There are several trend modelling approaches that have gained popularity in practice, mainly as a result of their ease of application:

1. Hand contouring of geologic sections accounting for drillhole data and analogue information.

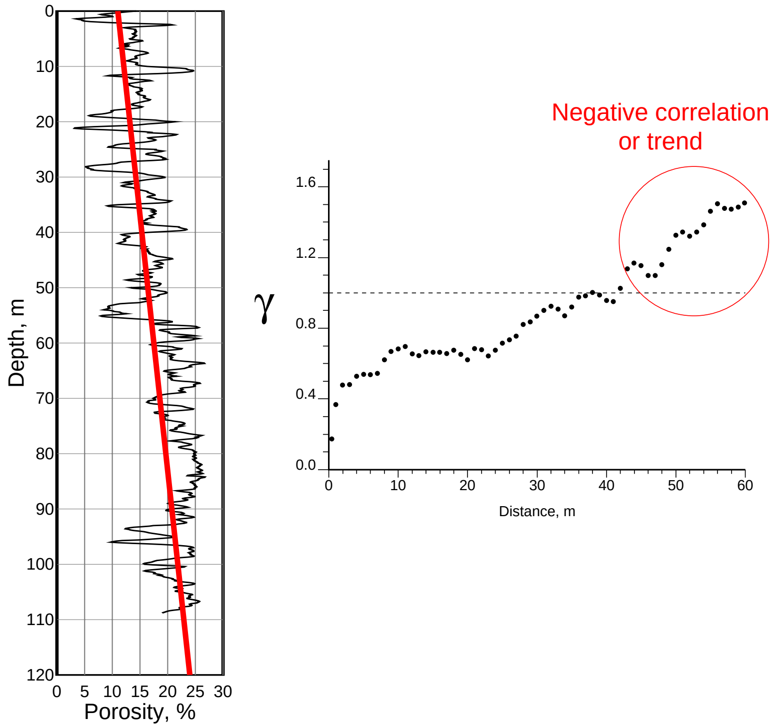

Figure 2: Example of porosity log (left) and corresponding vertical variogram (right) showing existence of a vertical trend.

2. Calculate moving window averages at each location and use this smooth map as a trend map.

3. Apply common robust estimation algorithms such as ordinary kriging to generate a smooth trend map.

Universal kriging [5] or intrinsic random functions of order k (IRF-k) could also be considered for automatic modelling of the trend. Typically a low order (≤ 2) polynomial function is used to model the trend (a polynomial of order 0 amounts to ordinary kriging with an unknown local mean) [6]. Automatic fitting of the trend using polynomials is generally not recommended as extrapolation of the trend may give rise to unrealistic grades or petrophysical properties. The use of these methods in simulation is problematic and not implemented in most software.

Another common approach to constructing a 3-D trend model is to develop a 1-D and a 2-D trend model and integrate these into a consistent 3-D trend model. A 1-D vertical trend could be developed to capture the trend within drillholes. A 2-D trend map in the horizontal plane could be used to capture any areal trends that may exist between the drillholes. There is no unique way to integrate these two trends into a consistent 3-D trend model [2]; however, one such approach is to scale the areal trend by the proportion of the vertical trend to the global mean:

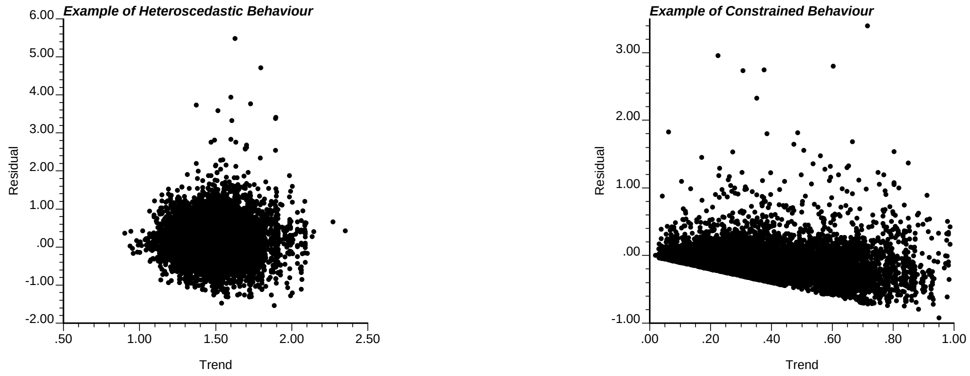

Figure 3: Example of heteroscedastic variance of residuals (left), and linear constraint on residuals (right).

$$m(x, y, z) = m_{global} \cdot \left(\frac{m(z)}{m_{global}} \right) \cdot \left(\frac{m(x, y)}{m_{global}} \right) \quad (3)$$

This is straightforward and well adapted to practice where limited data may make it difficult to infer a full 3-D trend model. Inherent in Equation 3 is an assumption of conditional independence of the vertical trend component within the horizontal plane and the horizontal trend component in the vertical direction.

Problems in Trend Decomposition

Given this common approach of decomposing the RV, the term "trend modelling" has come to be synonymous with the modelling of the local mean. Unfortunately, this is a rather limited view in the sense that trends may exist in both the mean and/or the variance. Common geostatistical estimation and simulation tools, with the exception of indicator approaches, implicitly assume homoscedasticity. Figure 3 (left) shows an example of a heteroscedastic relationship between the trend and the residuals. Straightforward application of geostatistical modelling does not account for these departures from stationarity; these must be explicitly handled in the construction of the numerical model of the residual random variable (RV).

The second problem arises as a consequence of the simple decomposition of the RV $Z(\mathbf{u})$ in Equation 1. Inevitably, this dissociation results in some constrained bivariate relationship between the trend component, $m(\mathbf{u})$, and the residual component, $R(\mathbf{u})$. For a non-negative RV $Z(\mathbf{u})$, the residual component must be greater than or equal to the negative trend component, that is, $R(\mathbf{u}) \geq -\mathbf{m}(\mathbf{u})$. Figure 3 (right) shows an example of this type of constraint for a copper deposit for which a 3D trend model was constructed.

The problem arises in the reproduction of this constraint feature after the residuals have been modelled and the trend must be added back to obtain the modelled value of $Z(\mathbf{u})$. A simple addition provides no assurance that $Z(\mathbf{u})$ will be non-negative at unsampled locations.

These two problems of trend modelling must be addressed in order to achieve the initial objectives of constructing numerical models that are geologically realistic and physically plausible.

Proposed Methodology

TThe idea is to complement the current practice of trend modelling by a transformation that accounts for both heteroscedastic and constraint behaviour.

The proposed transformation is a normal score transform of the residual data *conditional* to its trend component. Based on the probability class of the trend component, the corresponding residuals can be conditionally transformed:

$$Y_R(\mathbf{u}) = G^{-1}[F\{R(\mathbf{u}) \mid y_m(\mathbf{u})\}] \tag{4}$$

The result is a transformed residual distribution that is standard Gaussian. This transform effectively removes any heteroscedastic or constraint features that may be problematic in the modelling of the residual component.

Figure 4 shows a schematic illustration of this proposed transformation sequence. For practical purposes, mean values are partitioned into classes. Although the schematic shows only 3 classes, the number of classes should be at least 10 to 20 classes in practice. The minimum number of data should be large enough to give reliable conditional distributions.

Much like the forward transformation, the back transformation of the modelled residual values must be conditioned to its collocated trend value. Complex bivariate features are reproduced by way of the back transformation that respects the shape of the multiple conditional distributions.

Application

Implementation of the forward and backward transformation is straightforward. Two programs, `nscore_t` and `backtr_t`, were developed that are consistent with GSLIB convention [3].

Mining Example

The data used in this application was taken from a copper mine. Figure 5 shows the location map of the available drillholes alongside the crosssplot of Cu grade against elevation, which shows evidence of a vertical trend. The location map in Figure 5 also indicates a trend of high values in the northern half of the map. The trend model is constructed by first calculating a vertical trend. Secondly, a horizontal trend map must be generated to give a 2D trend. This involves calculating vertical averages across the horizontal domain from the data. Using these vertical averages, a 2D trend map can be generated by any of the common methods previously mentioned. For this data, the horizontal trend map will be created by kriging; Figure 6 shows the vertically averaged Cu data that is used as conditioning data in kriging alongside the resulting kriged map.

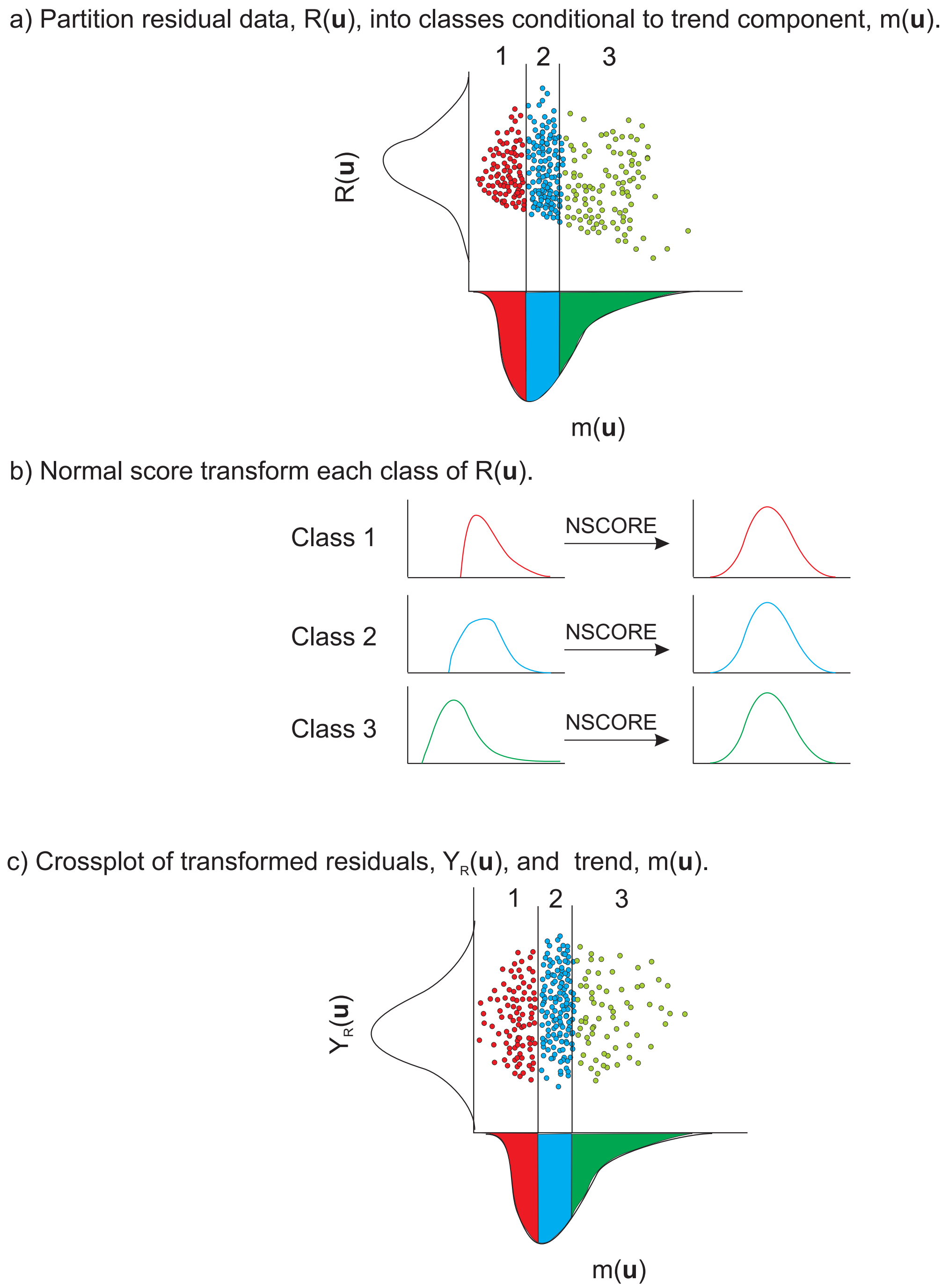

Figure 4: Normal score transform of residuals conditioned to trend component: (a) partition residuals into classes based on its trend component, (b) normal score transform each residual class, and (c) assemble all transformed residuals (from all classes) and plot against the trend to show bivariate distribution with homoscedasticity and approximately zero correlation. Note that the marginal distribution of $Y_R(\mathbf{u})$ is Gaussian.

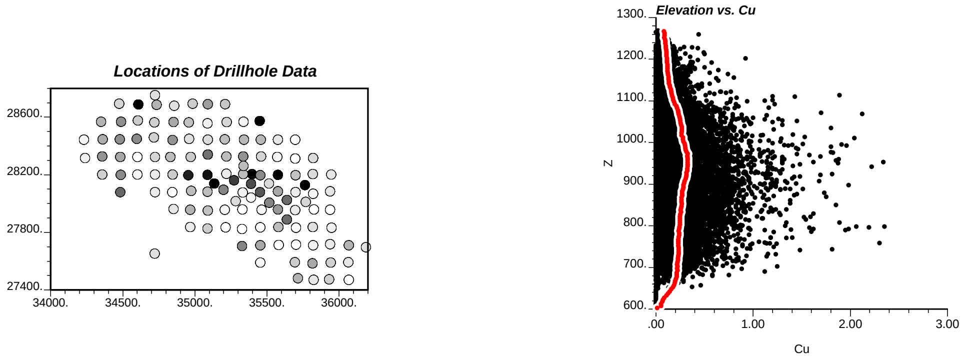

Figure 5: Location map of available drillholes (left) and crossplot of elevation vs. Cu to illustrate 1-D trend in the vertical direction (right).

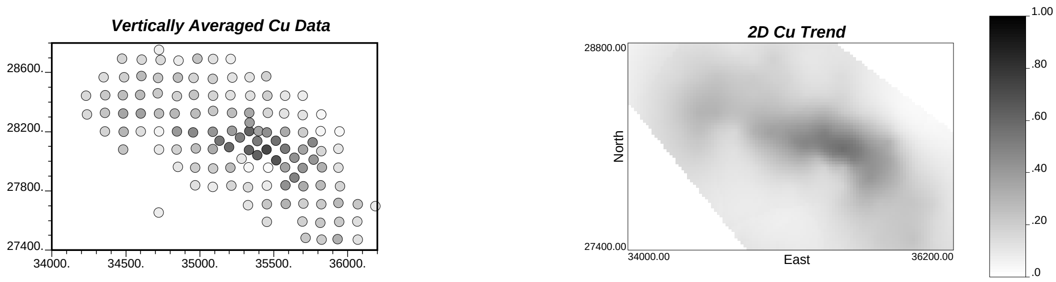

Figure 6: Location map of vertically averaged Cu data (left), and resulting kriged map using this data (right).

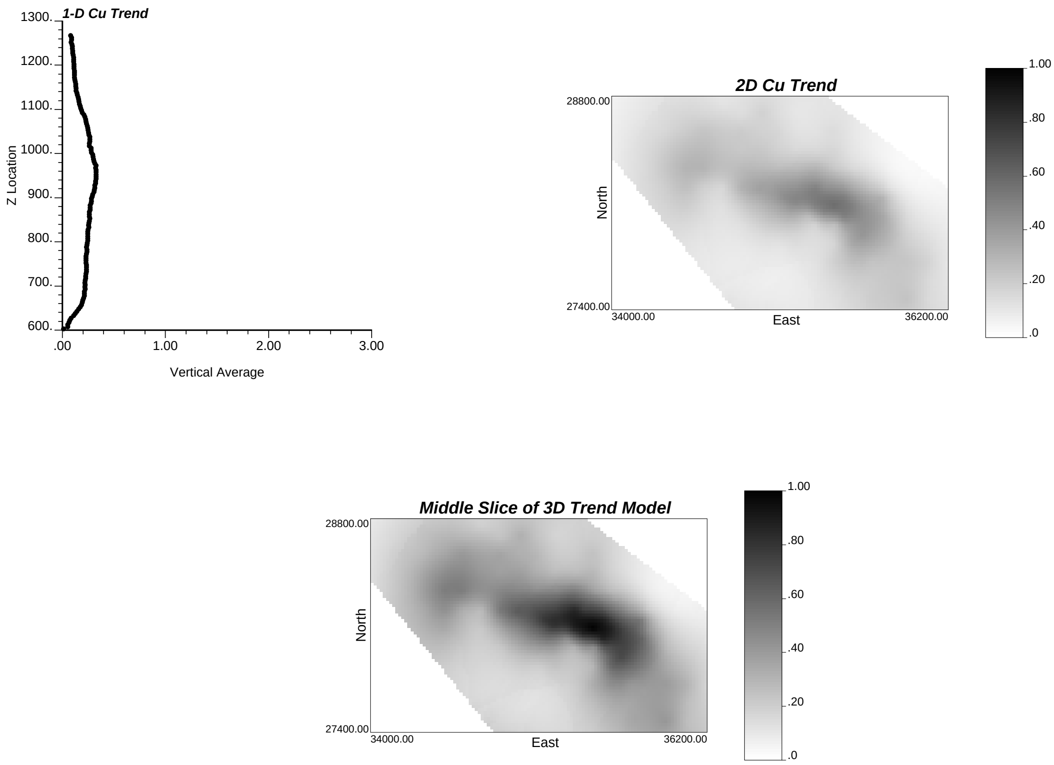

Figure 7: Required 1D trend (left) and 2D trend (middle) for integration to obtain 3D trend (right).

Regardless of the method chosen to create a 2D trend map, these lower dimension trends must still be integrated into a consistent 3D trend model. Using the 1D and 2D trends shown in Figures 5 and 6, Equation 3 was used to obtain a 3D trend model (see Figure 7).

Using the 3D trend model, the residuals are calculated using Equation 1. The resulting relation between the trend and the residual is captured in a crossplot shown in Figure 8. Clearly, a constraint is imposed on the residual values as a consequence of the trend model and non-negative grade values. Modelling the residual values to obtain a 3D residual model must reproduce this constraint relationship with the trend in order to obtain non-negative model values of the Cu grade.

To simulate the residuals, sequential Gaussian simulation will be used. Applying the conventional normal score transform to the residuals yields the crossplot shown in Figure 9. Figure 9 clearly shows the transference of the linear constraint in original space (see Figure 8) to an almost linear constraint in normal space. The correlation between the mean and transformed residual is -0.305, significant enough to indicate that the two RVs should be modelled in a dependent fashion. Further, the use of popular Gaussian simulation techniques would not be able to reproduce this type of constraint, regardless of whether kriging or cokriging is used.

The conditional normal score transformation of the residuals is then performed, and the corresponding histograms and crossplot are shown in Figure 10. The transformed residuals

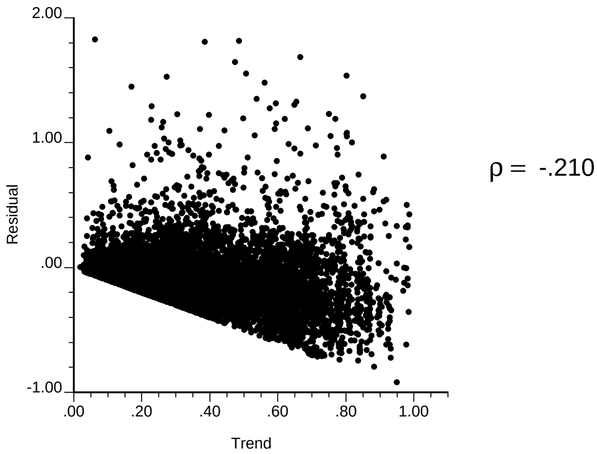

Figure 8: Linear constraint on residual values due to trend component.

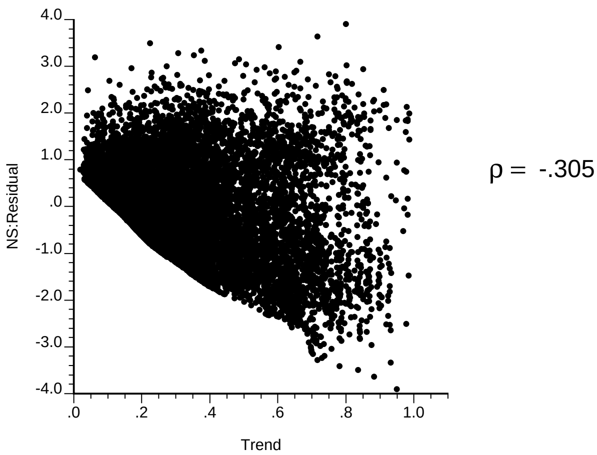

Figure 9: Crossplot of transformed trend vs. transformed residual using the conventional normal score transform on both RVs.

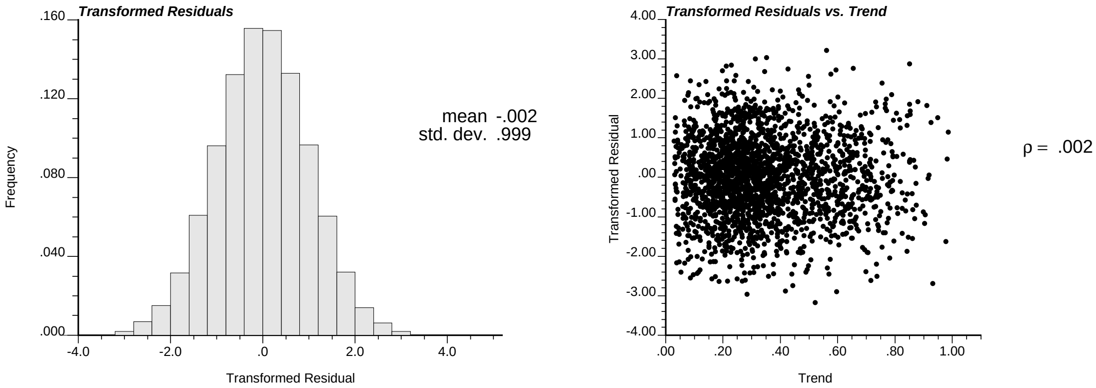

Figure 10: Histogram of transformed residual (left) and crossplot of normal score transformed trend vs. the conditionally transformed residual components (right).

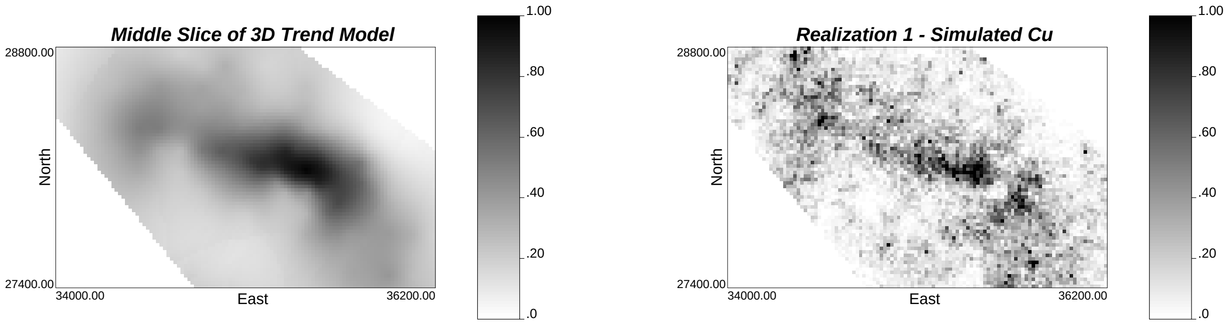

Figure 11: Comparison of trend model (left) and simulated realization of Cu (right), after adding the trend back to the simulated residuals.

are univariate Gaussian, and the constraint features have been removed. Further, the zero correlation combined with homoscedasticity of the resulting bivariate distribution permits independent simulation of the transformed residuals.

Variography and simulation of the conditionally transformed residuals are then performed. Following simulation, the simulated residuals are back transformed. Then, the trend model shown in Figure 7 is added to each of the residual realizations to obtain multiple realizations of Cu. One simulated realization of Cu is shown in Figure 11.

Figure 12 shows the comparison of the distribution of the first realization of simulated Cu and the declustered histogram of the original Cu data. The summary statistics are comparable, as is the shape of the distribution; however, negative values are apparent in the distribution of the simulated Cu.

Negative grades in the simulated Cu values must also be examined. In the first realization, 37 444 of the 817 400 blocks simulated yielded slightly negative Cu grades after the trend and residuals models were added due to imprecision in the classes. This amounts to 4.6 % of the modelled blocks. In comparison, the conventional normal score approach

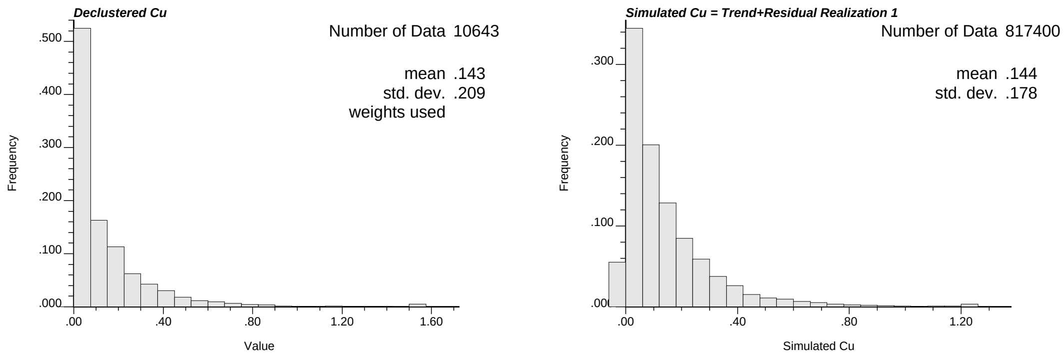

Figure 12: Comparison of declustered Cu distribution (left) with the first realization of simulated Cu, after adding the trend component to the simulated residuals (right).

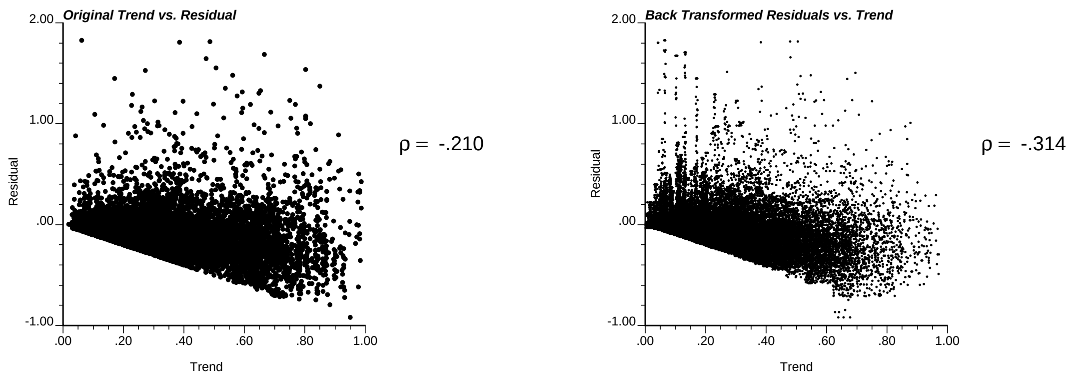

Figure 13: Comparison of original trend-residual crossplot and modelled trend - simulated residual crossplot. Notice that the linear constraint from the original crossplot is reproduced.

yielded 250 856 negative valued blocks or 30.7 %. The conditional transformation approach provides an obvious improvement from the conventional approach. In fact, all 37 444 negative values fall within the last probability class as specified by a trend value of 0.62. This is consistent with the small group of points in the bottom right corner of Figure 13 of the simulated values (right figure).

The real test in this exercise is actually the reproduction of the bivariate relation between the residual and its collocated trend value. This is shown by plotting a single realization of the residuals with the 3D trend model; Figure 13 reveals that the linear constraint is reproduced. In contrast, the standard normal score approach produced the crossplot shown in Figure 14. Clearly the linear constraint is not reproduced by the conventional transform.

Petroleum Example

Figure 15 shows the location map of the available 63 wells and the 1D vertical trend in the well log porosity. Note that for this example, an exaggerated 100:1 stratigraphic coordinate is used.

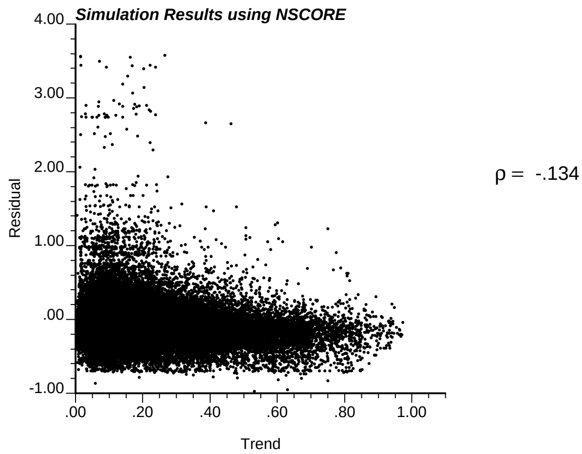

Figure 14: Crossplot of the modelled trend vs. simulated residuals from applying the conventional normal score transform. The linear constraint from the original crossplot is not reproduced.

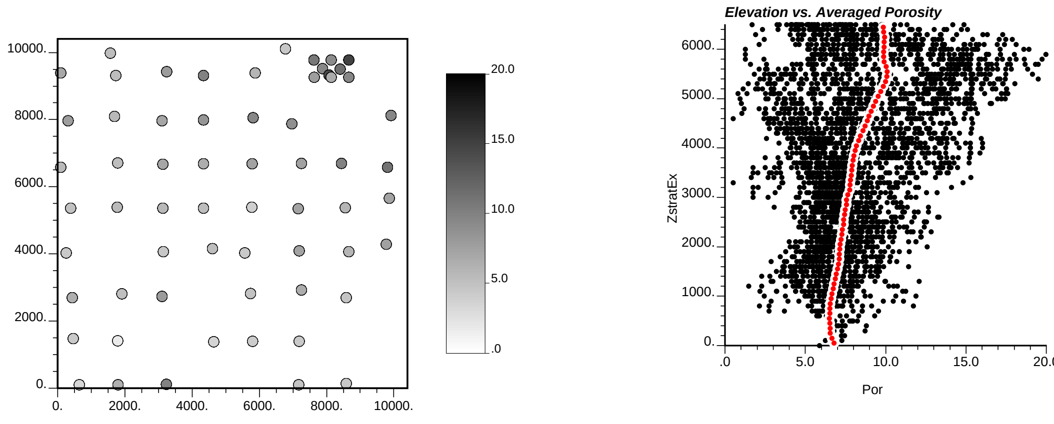

Figure 15: Location map of available wells (left) and crossplot of elevation vs. core porosity to illustrate 1-D trend in the vertical direction (right). Note that a 100:1 exaggerated vertical scale is applied.

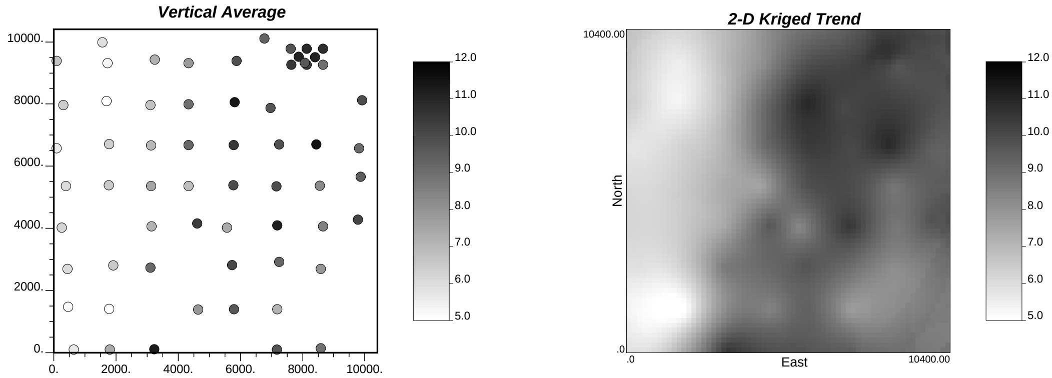

Figure 16: Location map of vertically averaged porosity data (left) and resulting areal trend map using this data (right).

Similar to the previous mining example, the data are averaged vertically at each well location to yield 63 conditioning data. These data are input to a 2D kriging to give an areal trend model (Figure 16).

Equation 3 is implemented to integrate the 1D and 2D trends from Figures 15 and 16 into a consistent 3D trend model (Figure 17).

Using this trend model, the residuals are calculated. A crossplot between these residuals and the collocated trend values shows the resulting non-linear relationship (Figure 18). Note that although the correlation coefficient is close to zero (0.019), this value only refers to the *linear* relationship and does not adequately reflect any non-linear features.

The proposed transformation is applied and the resulting histogram of the transformed residuals and its relation to the transformed trend component are shown in Figure 19. These transformed residuals are then simulated and back transformed. The 3D trend model is then added to the resulting realizations to obtain multiple realizations of porosity. Figure 20 provides a comparison of the 3D trend model and one realization of simulated porosity. It shows the reproduction of the large scale features captured by the trend model.

Finally, the histogram of the simulated porosity and the crossplot of the trend and the residual can be compared. Figure 21 shows the histogram reproduction of porosity. Figure 22 shows the comparison between the crossplot using the available data and the crossplot resulting from the simulated residuals and the trend model. There is good reproduction of both the univariate distribution and the complex bivariate non-linear features.

Conclusions

Trend modelling is an integral part of characterizing natural resources. Geostatistical methods rely on stationary statistics, which is counter-intuitive to most real reservoirs, mines or other naturally varying phenomena. Although common practices have been developed in the modelling of trends, none of these methods explicitly control the relation between the trend component and its collocated residual. This poses a problem since complex constraint, non-linear and heteroscedastic relations are common.

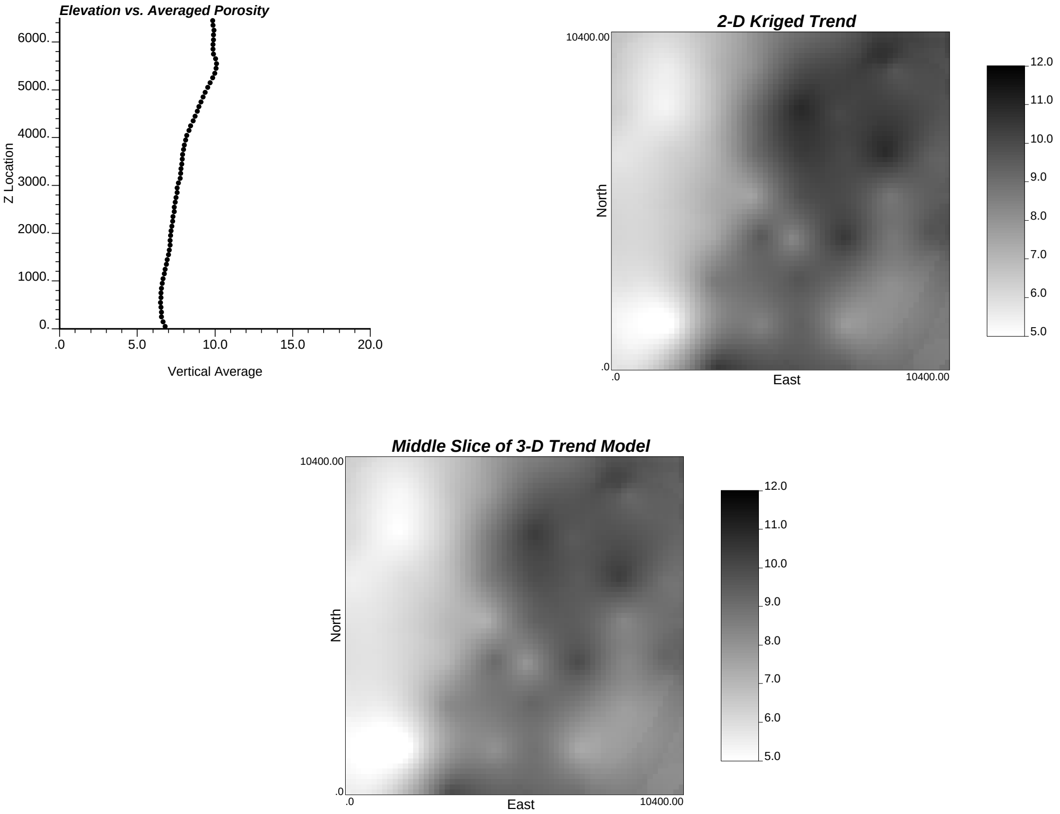

Figure 17: Required 1D vertical trend (top left) and 2D areal trend (top right) used to construct a 3D porosity trend (bottom).

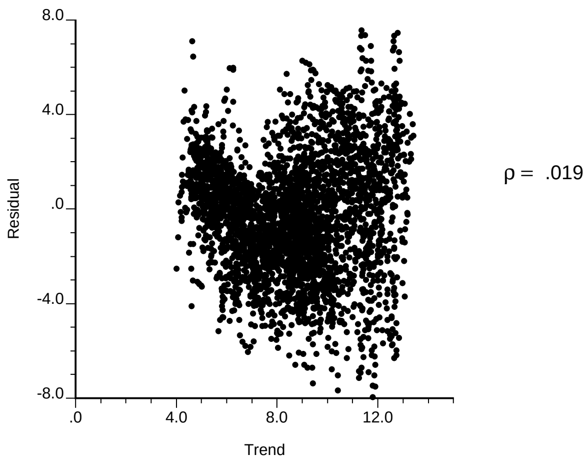

Figure 18: Relation between residual values and collocated trend component.

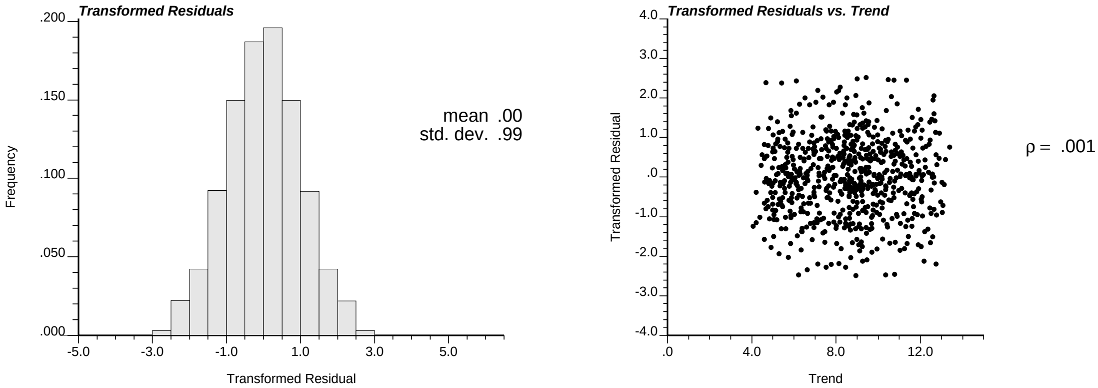

Figure 19: Histogram of transformed residual (left),and crossplot of normal score transformed trend vs. the conditionally transformed residual components.

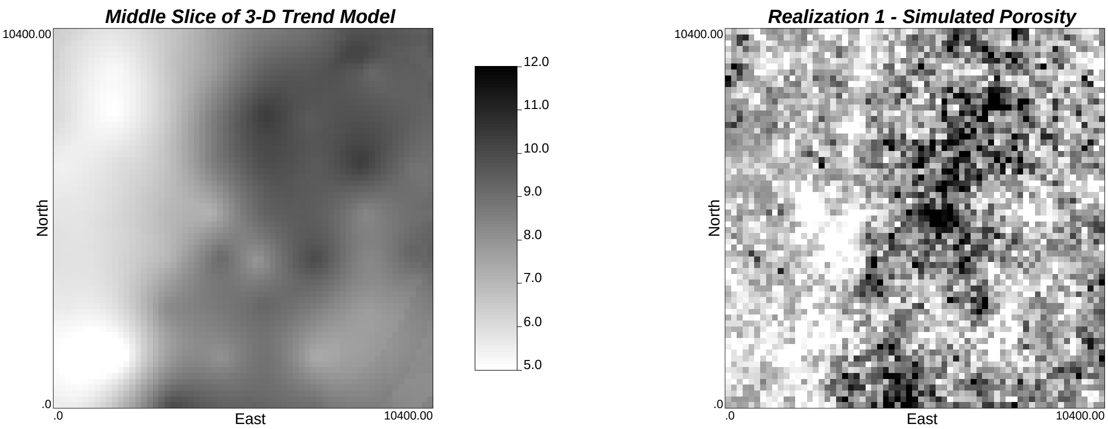

Figure 20: Comparison of trend model (left) and a realization of simulated porosity (right).

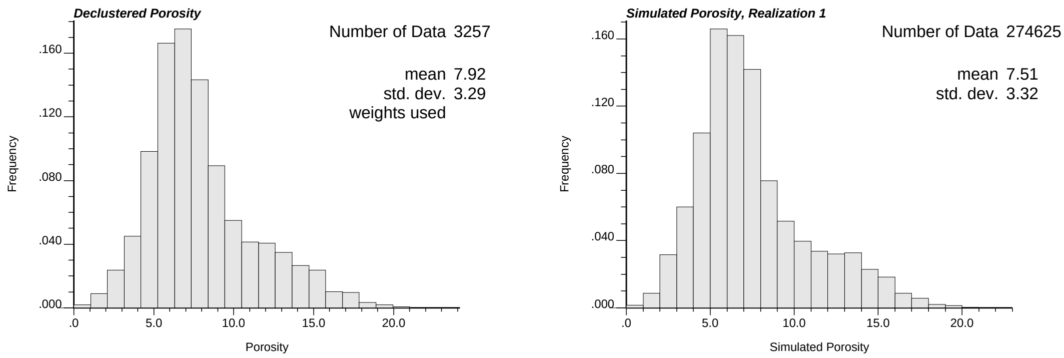

Figure 21: Comparison of declustered porosity distribution (left) with the first realization of simulated porosity (right).

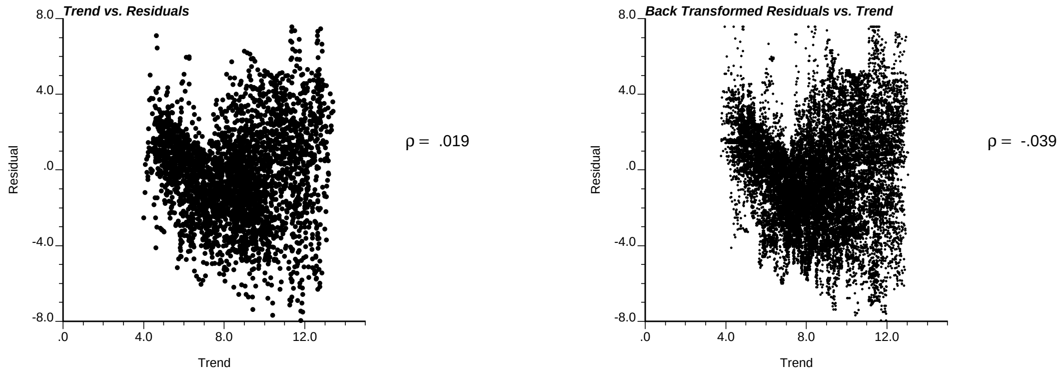

Figure 22: Comparison of original trend-residual crossplot and modelled trend - simulated residual crossplot. Notice that the non-linear features are reproduced.

A modified normal score transform for the residual is proposed that permits the application of Gaussian techniques, with the added advantage of reproducing complex relationships between the trend and the residuals. Applications to a Cu deposit and a petroleum reservoir are used to illustrate the robustness of the transform for detrended data.

Acknowledgements

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