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# Transformation of Residuals to Avoid Artifacts in Geostatistical Modelling With a Trend[1]

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*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. A petroleum-related application shows the robustness of the proposed transformation. Furthermore, a mining application shows that when this conditional transformation is applied to the original variable, instead of the residual, simulated values are assured to be nonnegative.*

**KEY WORDS:** trend modelling, stepwise conditional transformation, normal scores, sequential Gaussian simulation.

## 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 that 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,

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

where **u** and **h** are location and lag vectors, respectively, in domain $A$. For practical purposes, second-order stationarity is assumed explicitly for geostatistical

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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 an indepth treatment on stationarity for statistical inference, see Journal (1985).

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 dependent on the practitioner. Trends depend on many factors, including the available data 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 (RV) 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 (Fig. 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 to permit more reliable calculation of the local statistics (Goovaerts, 1997; Isaaks and Srivastava, 1989). 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.

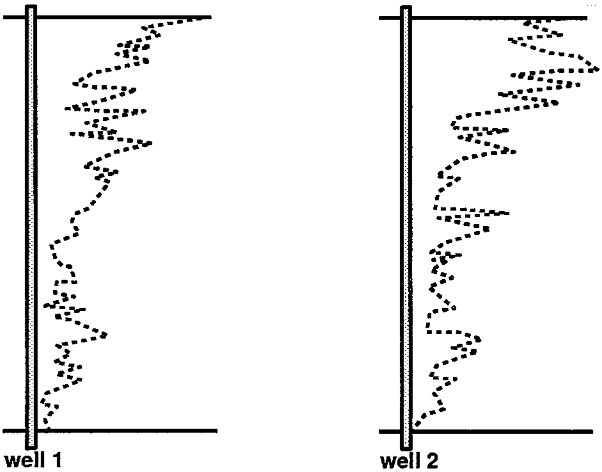


**Figure 1.** Example of vertical trend as indicated by two well logs (*Source*: Deutsch, 2002).

One further step is to examine the data for a proportional effect, that is, whether the local variance is dependent on the local mean (Journel and Huijbregts, 1978). 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 RV as the lag distance, **h**, increases (Fig. 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 RV into two components—the trend and the residual:

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

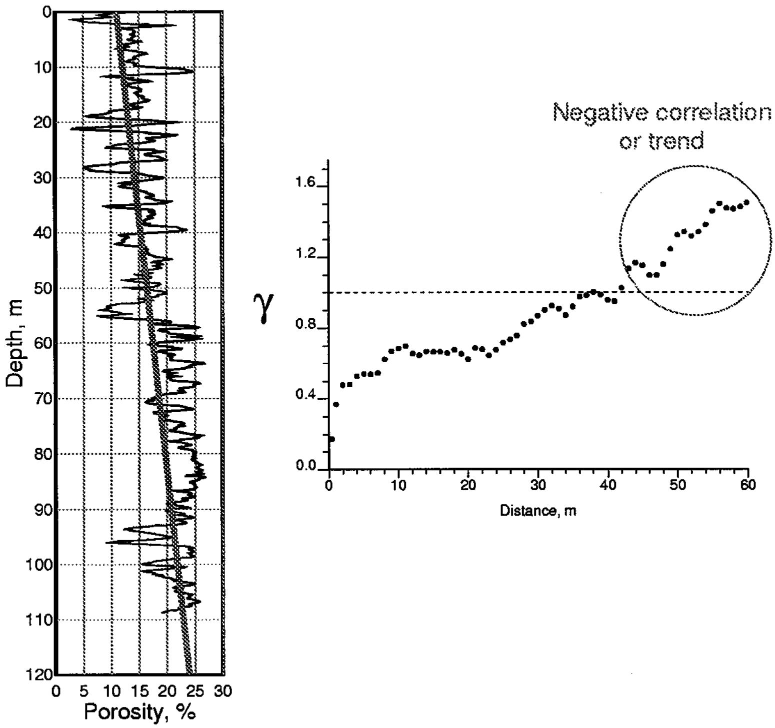


**Figure 2.** Example of porosity log (left) and corresponding vertical variogram (right) showing existence of a vertical trend.

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 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 $\sigma_Z^2$ is the variance of the original RV, $\sigma_R^2$ 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 (Deutsch, 2002).

The mean component is defined at all locations via a three-dimensional (3-D) trend model, while the residual values are only defined at data locations. 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 (Journel and Rossi, 1989).

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 data and analogue information.
2. Calculate moving window averages.
3. Apply common robust estimation algorithms such as ordinary kriging to generate a smooth trend map.

Universal kriging (Huijbregts and Matheron, 1971) or intrinsic RFs of order $k$ (IRF-$k$) could also be considered for automatic modelling of the trend. Typically a low-order ($\leq 2$) polynomial function is used to model the trend (a polynomial of order 0 amounts to ordinary kriging with an unknown local mean) (Isaaks and Srivastava, 1989). 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 is not implemented in most software.

Another common approach to constructing a 3-D trend model is to develop a one-dimensional (1-D) and a two-dimensional (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 drill holes. A 2-D trend map in the horizontal plane could be used to capture any areal trends that may exist between the drill holes. There is no unique way to integrate these two trends into a consistent 3-D trend model (Deutsch, 2002); however, one approach is to scale the areal trend by the proportion of the vertical trend to the global mean:

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

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.

Much like trend detection, trend modelling is also subjective. The approaches listed above provide numerous ways to model a trend, but the choice of the appropriate method depends on expert geological knowledge of the depositional environment and expert interpretation of the available data.

## Problems in Trend Decomposition

Given this common approach of decomposing 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 RV.

The second problem arises as a consequence of the simple decomposition of 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 nonnegative RV $Z(\mathbf{u})$, the residual component must be greater than or equal to the negative trend component, that is, $R(\mathbf{u}) \geq -m(\mathbf{u})$. Figure 3 (right) shows an example of this type of constraint for a copper deposit with a 3-D trend model.

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 nonnegative at unsampled locations.

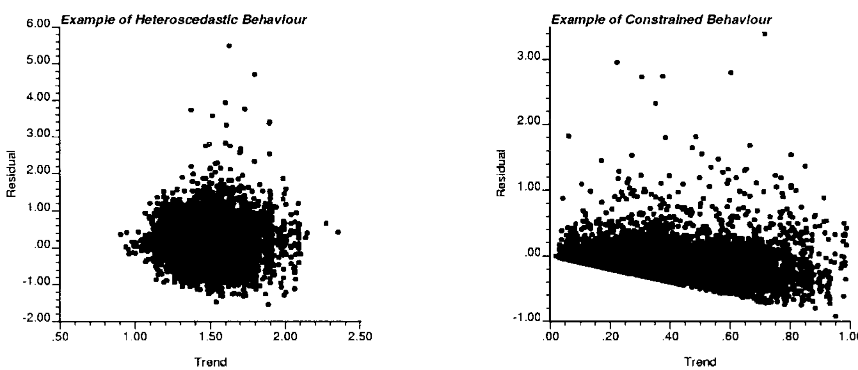


**Figure 3.** Example of heteroscedastic variance of residuals (left) and linear constraint on residuals (right).

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

## PROPOSED METHODOLOGY

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

The proposed transformation is a normal score transform of the residual data *conditional* to its trend component. On the basis of the probability class of the trend component, the corresponding residuals can be conditionally transformed (Leuangthong and Deutsch, 2003; Luster, 1985; Rosenblatt, 1952):

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

where the RV $Y_R$ indicates the Gaussian transform of the residual RV, $G^{-1}$ is the inverse Gaussian equation, and $F$ denotes the cumulative distribution function. 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 three classes, in practice the number of classes should be at least 10–20 classes to effectively remove the complex features. 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.

Further, the same transform can be performed on the *original variable* rather than the residual variable, $R$. This amounts to transforming the original variable, $Z$, conditional to the collocated trend component:

$$Y_Z(\mathbf{u}) = G^{-1}[F\{Z(\mathbf{u})|m(\mathbf{u})\}] \tag{5}$$

This alternative application of the same transform methodology is most effective when simulation may yield negative grades or petrophysical properties; one clear indication is the presence of a linear constraint in the trend–residual relationship, such as that shown in Figure 3. This resolves the issue of negative grades since the distribution of the original variable consists of only nonnegative

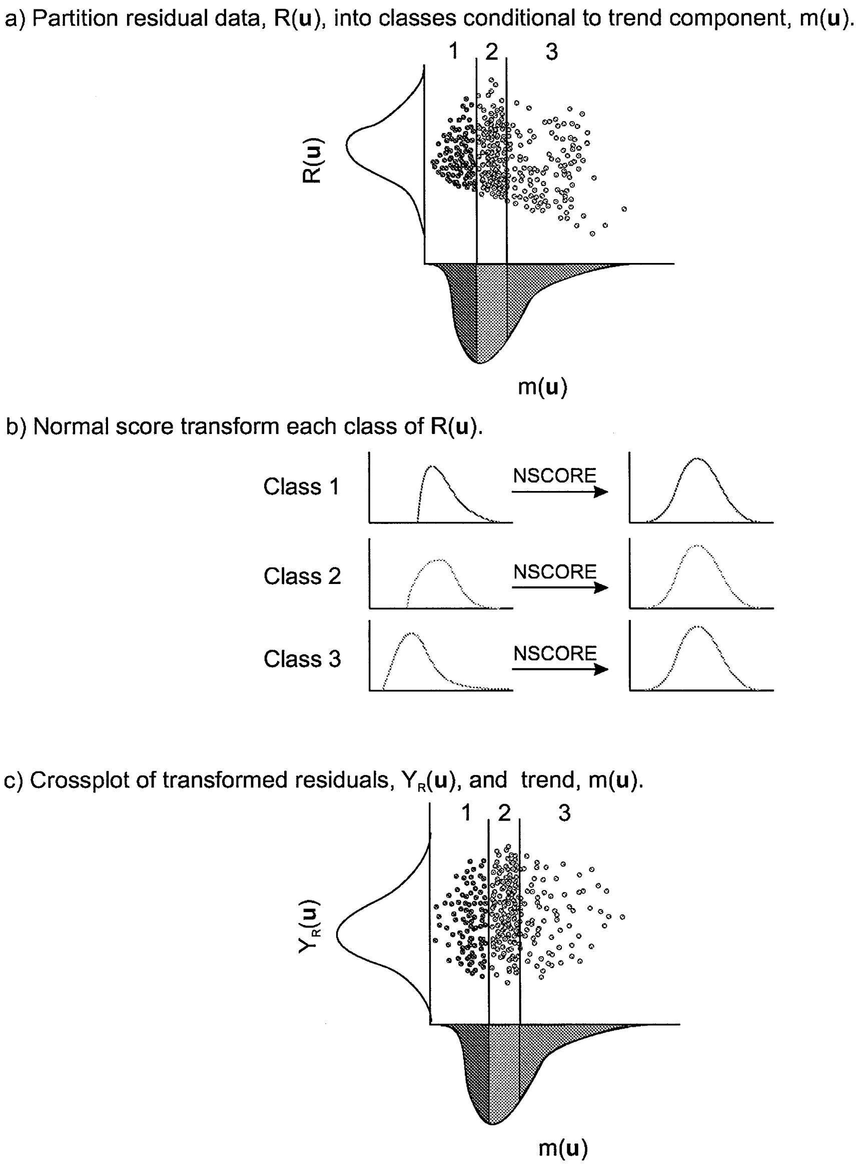


**Figure 4.** Normal score transform of residuals conditioned to trend component: (a) partition residuals into classes based on its trend component, (b) normal score transform each residual class, and (c) assemble all transformed residuals (from all classes) and plot against the trend to show bivariate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

values; thus, there is no possibility to back transform to a negative value, and hence no need to recode negative values to some artificial zero values for practical purposes.

## 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 (Deutsch and Journel, 1998).

Two applications are presented: petroleum and mining related. The former illustrates the ability of the transform to reproduce complex nonlinear, heteroscedastic features, while the latter shows the reduction of negative values in the presence of a linear constraint. Also shown in this latter example is an alternative application of the proposed transform to the original variable, rather than the residual variable; this removes all possibility of obtaining negative grades.

### Petroleum Example

Figure 5 shows the location map of the available 63 wells and the 1-D vertical trend in the well log porosity. Note that, for this example, an exaggerated 100:1 stratigraphic coordinate is used.

The trend model is constructed by first calculating a vertical trend. Secondly, a horizontal trend map must be generated to give a 2-D trend. This involves calculating a vertical average at each of the 63 well locations. Using these vertical averages, a 2-D trend map can be generated by any of the common methods previously mentioned. For this data, the horizontal trend map is created by kriging

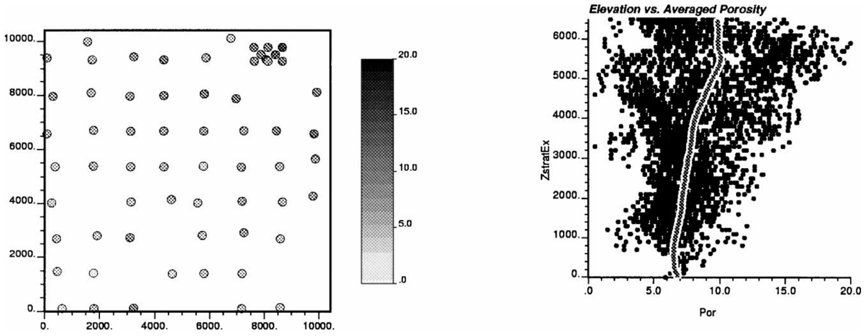


**Figure 5.** Location map of available wells (left) and crossplot of elevation vs. core porosity to illustrate 1-D trend in the vertical direction (right). Note that a 100:1 exaggerated vertical scale is applied.

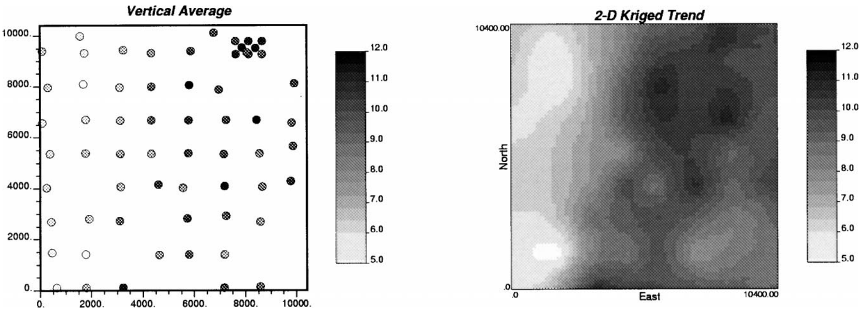


**Figure 6.** Location map of vertically averaged porosity data (left) and resulting areal trend map using this data (right).

(Fig. 6). Regardless of the method chosen to create a 2-D trend map, these lower dimension trends must still be integrated into a consistent 3-D trend model. Equation 3 is used to integrate the 1-D and 2-D trends from Figures 5 and 6 into a consistent 3-D trend model (Fig. 7).

Using this trend model, the residuals are calculated. A crossplot between these residuals and the collocated trend values shows the resulting nonlinear, heteroscedastic relationship (Fig. 7). 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 nonlinear features.

The proposed transformation is applied and the resulting histogram of the transformed residuals and its relation to the trend component are shown in Figure 8. The transformed residuals are univariate Gaussian, and the nonlinear and heteroscedastic features have been removed.

Variography and simulation of the conditionally transformed residuals are then performed. Following simulation, the simulated residuals are back

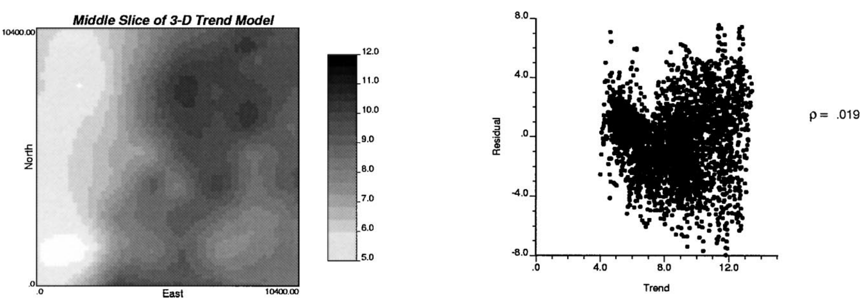


**Figure 7.** A cross section of the 3-D porosity trend (left) and the resulting relation between residual values and the corresponding trend component (right).

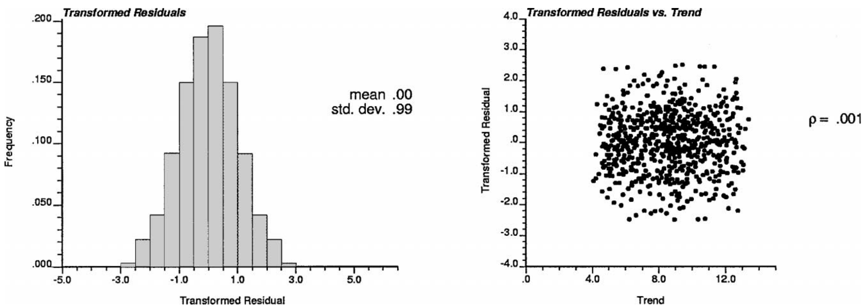


**Figure 8.** Histogram of transformed residual (left) and crossplot of normal score transformed trend vs. the conditionally transformed residual components.

transformed. The 3-D trend model is then added to the resulting realizations to obtain multiple realizations of porosity. Figure 9 provides a comparison of the 3-D 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 10 shows the histogram reproduction of porosity for one arbitrarily chosen realization. Figure 11 shows the reproduction of the bivariate distribution of the residuals and the trend. There is good reproduction of both the univariate distribution and the complex bivariate nonlinear features.

## Mining Example

The data used in this application was taken from a copper mine. Figure 12 shows the location map of the available drill holes alongside the crosssplot of Cu grade against elevation, which shows evidence of a vertical trend. The location

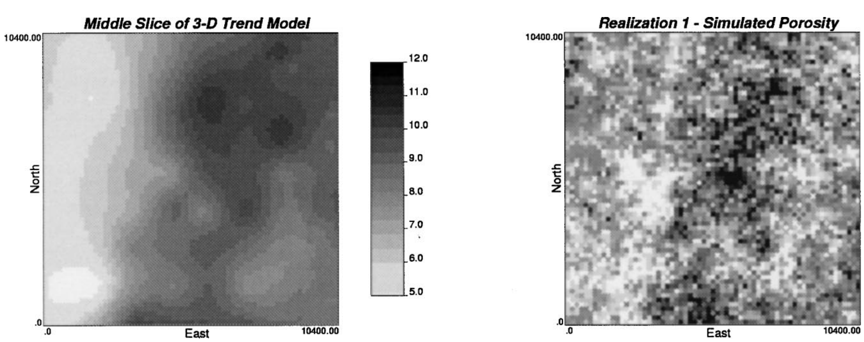


**Figure 9.** Comparison of trend model (left) and a realization of simulated porosity (right).

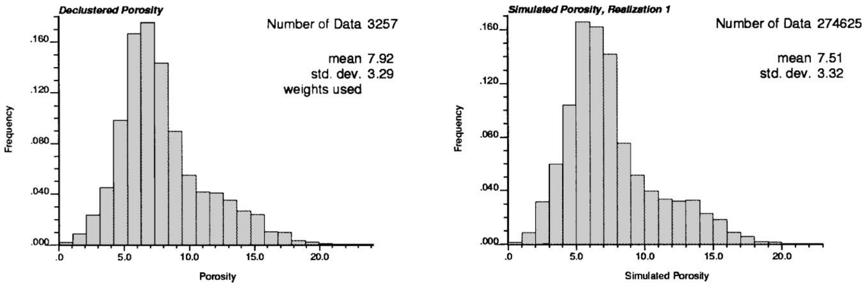


**Figure 10.** Comparison of declustered porosity distribution (left) with the first realization of simulated porosity (right).

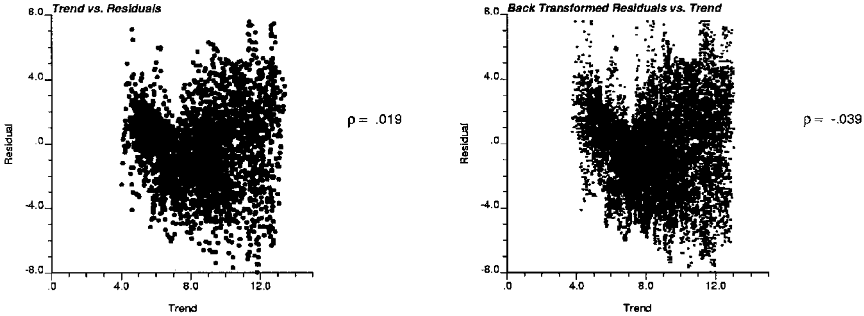


**Figure 11.** Comparison of original trend–residual crossplot and modelled trend–simulated residual crossplot. Notice that the nonlinear features are reproduced.

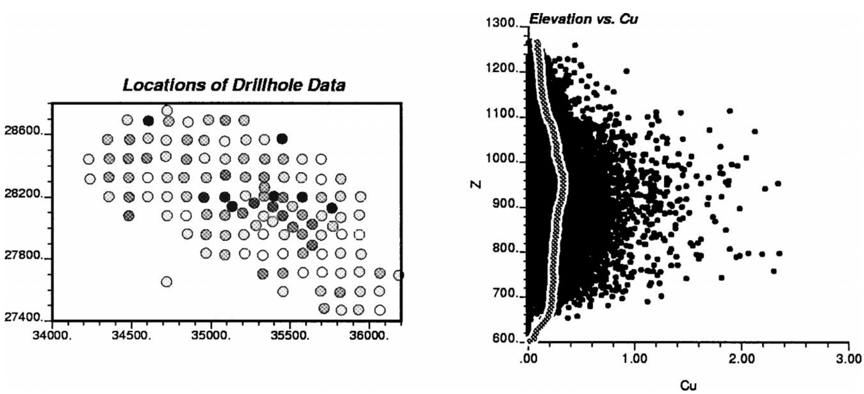


**Figure 12.** Location map of available drill holes (left) and crossplot of elevation vs. Cu to illustrate 1-D trend in the vertical direction (right).

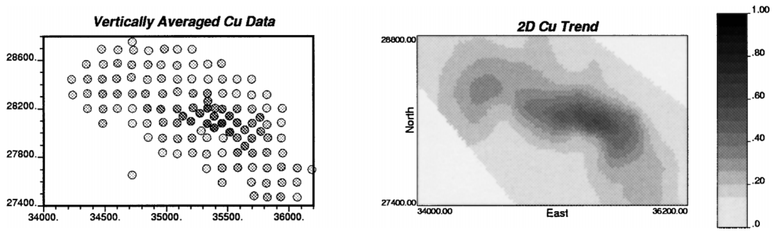


**Figure 13.** Location map of vertically averaged Cu data (left) and resulting kriged map using this data (right).

map in Figure 12 also indicates a trend of high values in the center of the map. Similar to the previous petroleum example, the data are averaged vertically at each drill hole location to yield conditioning data. These data are input to a 2-D kriging to give an areal trend model (Fig. 13). Using the 1-D and 2-D trends shown in Figures 12 and 13, Equation 3 was used to obtain a 3-D trend model (Fig. 14).

Using the 3-D trend model, the residuals are calculated using Equation 1. The resulting relation between the trend and the residual is captured in a cross-plot shown in Figure 14. Clearly, a constraint is imposed on the residual values as a consequence of the trend model and nonnegative grade values. Modelling the residual values to obtain a 3-D residual model must reproduce this constraint relationship with the trend to obtain nonnegative 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 cross-plot shown in Figure 15. Figure 15 clearly shows that the linear constraint in original space (Fig. 14) appears as 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.

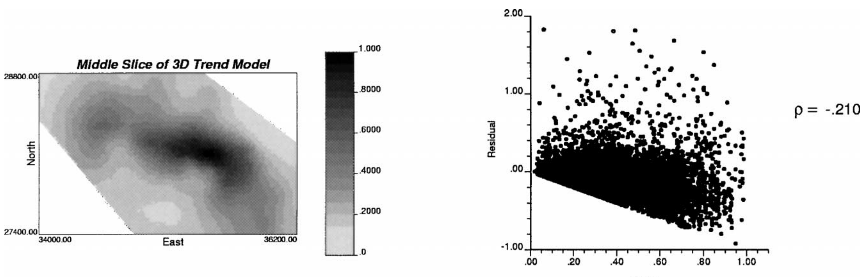


**Figure 14.** A cross section of the 3-D Cu trend (left) and the resulting linear constraint on residual values due to the trend component (right).

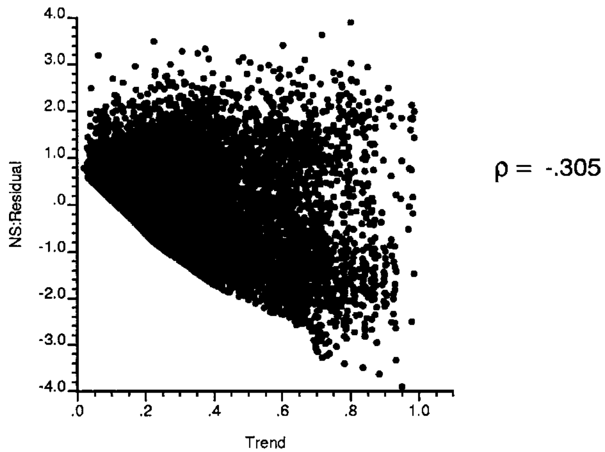


**Figure 15.** Crossplot of transformed trend vs. transformed residual using the conventional normal score transform on both RVs.

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 16. The transformed 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.

These transformed residuals are then simulated and back transformed. Then, the trend model (Fig. 14) is added to each of the residual realizations to obtain

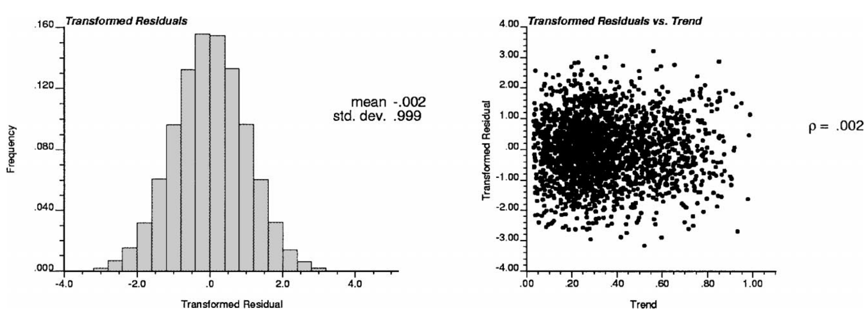


**Figure 16.** Histogram of transformed residual (left) and crossplot of normal score transformed trend vs. the conditionally transformed residual components (right).

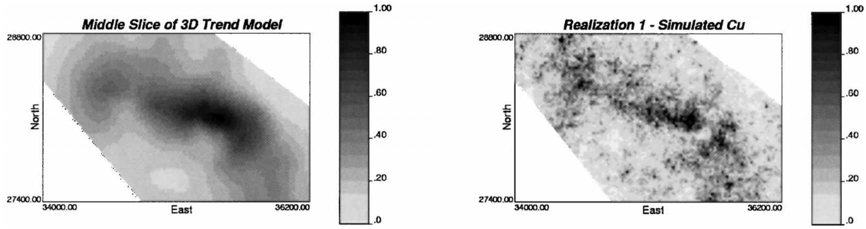


**Figure 17.** Comparison of trend model (left) and simulated realization of Cu (right), after adding the trend back to the simulated residuals.

multiple realizations of Cu. One simulated realization of Cu is shown next to the trend model in Figure 17.

Figure 18 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.

Reproduction of the bivariate relation between the residual and its collocated trend value is illustrated by plotting a single realization of the residuals with the 3-D trend model; Figure 19 reveals that the linear constraint is reproduced. In contrast, the standard normal score approach produced the crossplot shown in Figure 20. Clearly the linear constraint is not reproduced by the conventional transform.

A closer examination of negative grades in the simulated Cu values is required. In one realization, 37,444 of the 817,400 blocks simulated yielded slightly negative Cu grades after the trend and residuals models were added because of imprecision in the classes. This amounts to 4.6% of the modelled blocks. In comparison, the conventional normal score approach 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

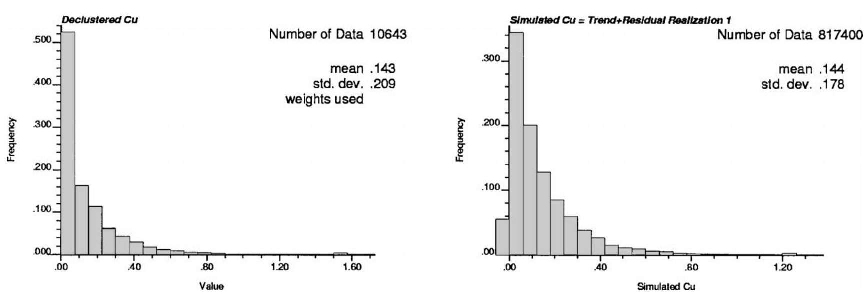


**Figure 18.** Comparison of declustered Cu distribution (left) with the first realization of simulated Cu, after adding the trend component to the simulated residuals (right).

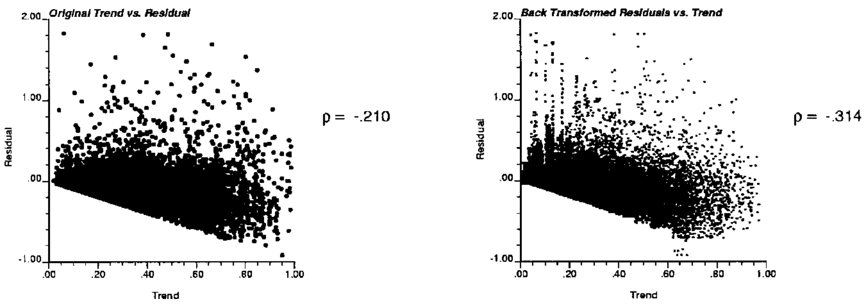


**Figure 19.** Comparison of original trend–residual crossplot and modelled trend–simulated residual crossplot. Notice that the linear constraint from the original crossplot is reproduced.

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 19 of the simulated values (right figure).

To avoid the possibility of obtaining negative simulated values, the transform was applied to the original Cu variable instead of the residual variable. The simulation and back transform are performed. The histogram of simulated Cu (Fig. 21) clearly shows that the target distribution is reproduced and there are no negative values. A realization of simulated Cu using the transformed original variables is compared to a realization using the transformed residual variables (Fig. 22). Both simulation results reproduce the large-scale features from the trend model, but

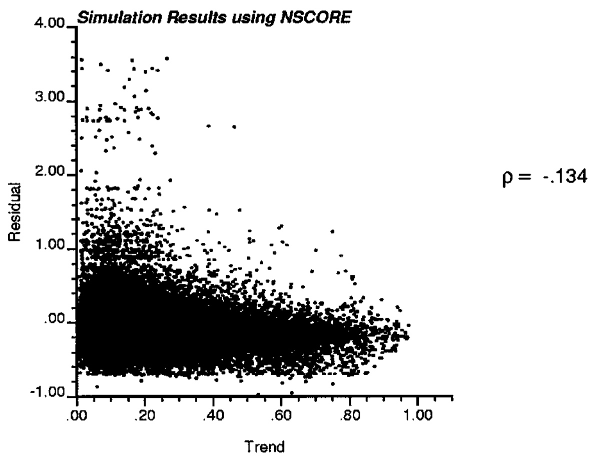


**Figure 20.** Crossplot of the modelled trend vs. simulated residuals from applying the conventional normal score transform. The linear constraint from the original crossplot is not reproduced.

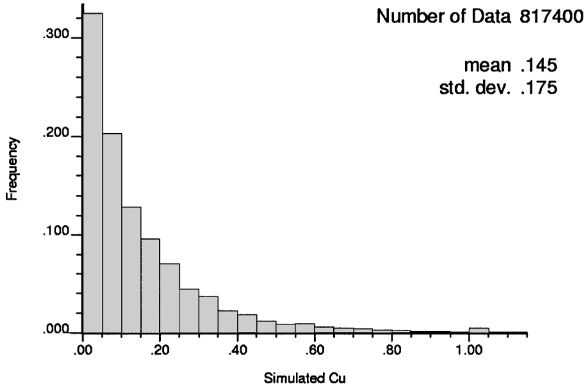


**Figure 21.** Distribution of simulated Cu values, resulting from applying transform to original Cu values conditioned to the trend. Note that the minimum simulated value is 0.0; simulation using this transform did not yield negative values.

the simulation results using the transformed original variable yield nonnegative values.

## CONCLUSIONS

Trend modelling is an integral part of characterizing natural resources. Geostatistical methods rely on stationary statistics, which is counterintuitive to most real reservoirs, mineral deposits, 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, nonlinear, and heteroscedastic relations are common.

A modified normal score transform for geostatistical Gaussian simulation of residual is proposed. The main idea is to transform the residual data conditional to

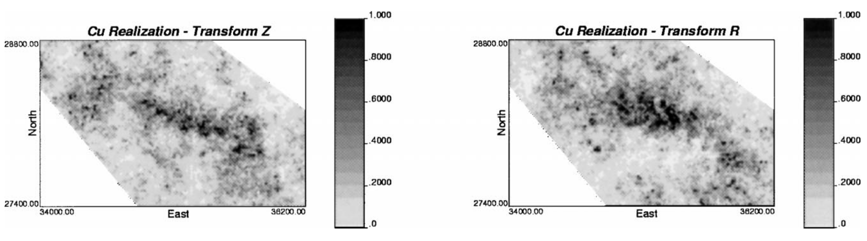


**Figure 22.** Comparison of a simulated realization (for the same random number seed) applying the conditional transform to the original variable, $Z$ (left) and to the residual variable, $R$ (right).

its corresponding trend component. This transform yields a transformed variable that is Gaussian and approximately uncorrelated to its trend. The conventional practice of independently simulating the residuals can then be performed. Back transformation conditional to the trend model permits reproduction of complex relationships between the trend and the residuals.

In the instance of nonlinear and heteroscedastic features, this transformation methodology can be applied on the residuals; however, for linear constraint features transformation of the residuals may still yield negative grades. For these cases, we propose transformation of the original variable conditioned to the trend, that is, model the original variable directly accounting for the trend model through the transformation. The mining application showed that all the simulated grades were nonnegative. This is a great advantage in that the need to recode negative values to some artificial zero value is completely avoided.

Although the proposed transformation allows us to account for one aspect of stationarity, there are many other aspects yet to be addressed. These include nonstationarity of the variogram, multivariate distribution, and the residual mean and variance. Future work is required to develop methodologies to account for these aspects.

Furthermore, two areas associated to the area of modelling in the presence of a trend remain important for future research. Firstly, the inference of the trend model is critical. The transformation proposed in this paper addresses the case of simulating the residuals or the original variable *after* the trend model has been constructed. More work in the preceding phase of building the trend is required. Secondly, after the trend model is built, inference of reliable statistics for the residual is an issue. The primary concern lies in the influence of the trend model on the statistics of the residuals, for instance, the overfitting of a trend could bias the statistics of the residuals. Of course, constructing an appropriate trend model and inferring reliable residual statistics are closely related areas of research.

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