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ORIGINAL PAPER

Detecting and quantifying sources of non-stationarity via experimental semivariogram modeling

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Abstract Conventional geostatistics often relies on the assumption of second order stationarity of the random function (RF). Generally, local means and local variances of the random variables (RVs) are assumed to be constant throughout the domain. Large scale differences in the local means and local variances of the RVs are referred to as trends. Two problems of building geostatistical models in presence of mean trends are: (1) inflation of the conditional variances and (2) the spatial continuity is exaggerated. Variance trends on the other hand cause conditional variances to be over-estimated in certain regions of the domain and under-estimated in other areas. In both cases the uncertainty characterized by the geostatistical model is improperly assessed. This paper proposes a new approach to identify the presence and contribution of mean and variance trends in the domain via calculation of the experimental semivariogram. The traditional experimental semivariogram expression is decomposed into three components: (1) the mean trend, (2) the variance trend and (3) the stationary component. Under stationary conditions, both the mean and the variance trend components should be close to zero. This proposed approach is intended to be used in the early stages of data analysis when domains are being defined or to verify the impact of detrending techniques in the conditioning dataset for validating domains. This approach determines the source of a trend, thereby facilitating the choice of a suitable detrending method for effective resource modeling.

Keywords Semivariogram · Non-stationarity · Mean trend · Variance trend

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1 Introduction

Trends are defined as low-frequency, large scale variations of a certain regionalized variable (Olea 1991). Here, the term 'trend' refers to large scale patterns in the local mean and/or local variance. Dealing with trends in the mean and/or variance is a longstanding challenge in mineral resource modeling. Mean trends are an important part of modeling natural resources (Leuangthong and Deutsch 2004). Extensive research has been conducted to deal with mean trends. Kriging estimators have been modified to account for mean trends by many authors such as Matheron (1969), Olea (1974), Davis and David (1978), and Costa (2009) among others. An iterative approach to filter the mean trend was proposed by Neuman and Jacobson (1984). Their approach resembles universal kriging, in that the mean trend is estimated from a set of functionals and its coefficients are iteratively estimated along with the inference of the residuals variogram. However, variance trends are not addressed. Journel and Rossi (1989) discussed the importance of accounting for trends and highlighted that different kriging approaches tend to give similar estimates when interpolating in densely sampled regions, with differences arising only when extrapolation is required in poorly sampled regions. In their analysis, trend models are fitted either by a local estimation of the mean value in ordinary kriging or the fitting through polynomials via kriging with a trend, usually retaining only low order monomials. There is no mention to variance non-stationarity and the issues of variogram estimation are addressed by finding a proper residual variogram or covariance, which in practice may not be simple. Furthermore, the global compensation of the kriging variance due to the presence of variance trends is disregarded as a problem.

While there is vast literature regarding non-stationarity in the mean, variance trends are often only mentioned in the presence of mean trends. These patterns of variability in the local standard deviation that are related to variations of the local mean are usually referred to as a proportional effect (Isaaks and Srivastava 1989; Manchuck et al. 2009). Detrending and/or data transformations are offered as possible solutions to mitigate the influence of a proportional effect in resource modeling.

In practice, domains are influenced by physical conditions that make it difficult to assume stationarity. The process of domaining when modeling mineral deposits relies on the geologic characterization of the information sampled by exploratory drilling campaigns. This characterization can be classified as generic or detailed depending on the geologist's criteria. A generic geologic interpretation is more restrictive for domaining because it tends to combine different rock types into a more generic rock type category. For example, magnetite exoskarn, garnet exoskarn and other types of exoskarn rock types may be characterized as simply exoskarn. On the other hand, a detailed interpretation better accounts for the heterogeneities in mineral grades, and gives more flexibility for defining larger domains because the various rock types interpreted can be combined into suitable stationary domains. In the case of generic geologic interpretations, mean and variance trends are more likely to be present. This poses a potential challenge for modeling using conventional geostatistical approaches, unless these trends are removed and residuals are modeled. Ignoring trends and applying conventional geostatistics can lead to:

- inflation of conditional variances;
- an incorrect definition of the corresponding semivariogram model; and
- compensation of the conditional variances over different regions in the domain, that is, over-estimation in some regions and under-estimation in others.

There are many approaches aimed at dealing with mean trends. One common approach considers decomposition of the original value into a mean component and a residual component (1):

$$R(\mathbf{u}) = Z(\mathbf{u}) - m(\mathbf{u}), \quad (1)$$

where $Z(\mathbf{u})$ represents the random variable (RV) in original scale units, $R(\mathbf{u})$ is the residual value after removing the mean trend, $m(\mathbf{u})$ is the mean trend and $\mathbf{u}$ is a location vector in $\mathbf{R}^n$. The mean trend component $m(\mathbf{u})$ is the expected value of $Z(\mathbf{u})$, hence, the residual $R(\mathbf{u})$ is centered at zero mean.

Classical approaches consist of calculating mean trends as smoothed models that are intended to capture the large scale variability of the mean in the domain. These models can be built using interpolation techniques such as moving window averaging or some kriging variants, and in the case of high dimensional trend models, they can be constructed by combining lower dimensional trends (McLennan 2007; Leuangthong et al. 2008). Also, the use of neural networks to obtain the mean trend has been proposed in Kanevski et al. (1996), and Demyanov et al. (2001) proposed the use of wavelets and frames for the same purpose.

David (1977) and Cressie (1985) discussed the use of relative semivariograms to account for variance trends that are proportional to the local means squared. Leuangthong and Deutsch (2004) proposed the use of stepwise conditional transformation for dealing with the residuals in presence of both the mean and variance trends. The trend in the variance is usually addressed as a consequence of the proportional effect that may be present in a domain because of the nature of the regionalized variable to be modelled. The proportional effect considers large scale dependences between local means and local variances in a domain or the dependence of mean and variances of two conditional distributions (Manchuck et al. 2009). However, the variability of the local variances in a domain can be independent to the variability of the local means, that is, mean trends are not necessarily related to variance trends. Underlying geologic structures rule the occurrence of the variable of interest in the domain. Consider a generic geologic characterization that combines two types of copper minerals in a domain, such as chalcopyrite and bornite. The former has less variability in copper grades compared to the latter. If the chalcopyrite mineralogy is dominant in one side of the domain and the bornite in the other with a soft transition in between, then there is a large scale pattern of variability of copper grades in the domain or a variance trend. In terms of a random function (RF), this is related to differences in the variance between regions of RVs (see Fig. 1d–f).

Two or more domains with different variability and the same mean should not be combined simply because there is

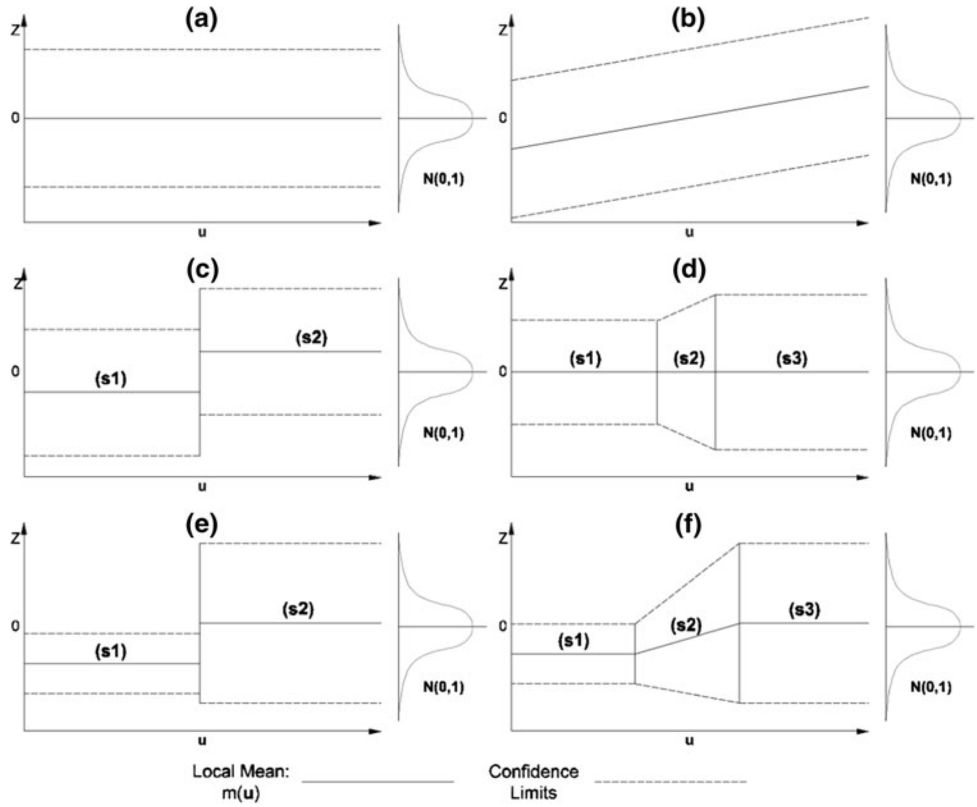


Fig. 1 Schematic 1D Gaussian environments: **a** constant local mean and local variance; **b** linear mean trend and constant local variance; **c** two sub-regions of constant local variance but different local means; **d** two regions of constant local mean but different local variance with a transition zone; **e** two sub-regions of different local means and different local variances; **f** two regions of different local means and different local variances with a transition zone; the *dashed lines* represent some confidence limits of the normal distributed RVs $Z(\mathbf{u})$

no mean trend. As in the case of mean trends, building geostatistical models in presence of variance trends can also have negative consequences. It is recommended to remove the variance trend after removing the mean trend; the latter could mask the variability in the domain since only one value is available at each location. A similar discussion is undertaken by Myers (1989). He gives an example of this by using a database of daily readings of SO_2, removing the mean trend by using increments, and the variance trends by means of a logarithmic transformation. Another approach to remove this trend is by standardizing the local variability (2):

$$Y(\mathbf{u}) = \frac{R(\mathbf{u})}{\sqrt{\sigma^2(\mathbf{u})}} \tag{2}$$

where $R(\mathbf{u})$ is the residual value after removing the mean trend, in original scale units with zero mean, $Y(\mathbf{u})$ is the standardized RV after removing the variance trend, and $\sigma^2(\mathbf{u})$ is the variance trend and $\mathbf{u}$ is a location vector in $\mathbf{R}^n$. The resulting variances of $Y(\mathbf{u})$ are all equal to one.

This paper proposes a method to identify and quantify the sources contributing to a trend by decomposing the experimental semivariogram into stationary and non-stationary components. These types of analysis are common and have been documented previously by other authors focussing mainly on mean trends, usually looking for a trend-free direction and assuming an isotropic behaviour of the residuals or modeling a local mean by some functional (Matheron 1969; Journel and Rossi 1989; Olea 2006). Still, there are a multitude of geomodeling methods and suggestions for dealing with trends related to the mean and/or the variance and the choice of which method is appropriate and effective for any particular setting is challenging. The proposed decomposition of the experimental semivariogram requires little additional effort for the geomodeler, with the added benefit of identifying the source of the trend contribution. The ability to identify whether the mean and/or the variance contributes to the non-stationarity of the deposit or reservoir feeds into a decision support system to determine an appropriate geomodeling approach to resource modeling.

2 Domaining for mineral deposits modeling

In conventional geostatistics, the semivariogram model is used to define the spatial continuity of a stationary random function (SRF). In practice, it is obtained by fitting the experimental semivariogram computed from the available dataset within a domain. This measure of spatial continuity is then used to infer metal or mineral grades or any attribute of interest at unsampled locations via estimation or simulation. A fundamental component of this framework is the decision of stationarity that permits the extraction of relevant statistics about the domain using only the available sampled data. Often, the assumption of second order stationarity, where the mean of the RVs and covariances of every two RVs separated by a common vector are considered to be constant, is sufficient for inference. However, in presence of a trend, the variogram is incorrectly estimated by the conventional approach, and should be inferred as a variance of the difference of the two RVs. A thorough discussion on the different types of stationarity often encountered in the literature and in practice can be found in Myers (1989), although this paper mainly discusses handling non stationarity by means of universal kriging and intrinsic random functions (IRFs) of order k (IRF-k).

Presence of mean trends is common in mineral deposits and results in a non-stationary environment (see Fig. 1b, c, e, f). Spatial variations in the local mean are captured by a semivariogram which increases rapidly and continues to do so beyond the sill (Chilès and Delfiner 1999). Domains without an apparent mean trend can still be non-stationary if the local variances are not constant. This condition is widely seen in practice when the variability of the variable of interest changes between regions within the proposed domain (see Fig. 1d–f).

In practice, domaining may be carried out using generic geologic characterizations. The resulting domains may be unsuitable for modeling using conventional geostatistics because of the presence of mean and variance trends. Even when the domain is assumed as stationary despite the presence of these trends, the estimated uncertainty parameters are inadequate for short and medium term mine planning which require a more accurate prediction or estimation of local uncertainty parameters.

When modelling a mineral deposit, transitions of variability of the regionalized variable between rock types can be hard or soft. A soft transition can be seen as an intermediate zone with gradual change in the local mean and/or in the local variance between two different sub-domains. On the other hand, a hard transition is an abrupt change in the local mean and/or local variance, usually present when the two sub-domains are independent of each other. Sketches of some possible transitions in a domain that are assumed to be multi-Gaussian are shown in Fig. 1. In case (a), the different rock types share the same local means and variances, making the domain suitable for modeling using conventional geostatistics. Case (b) shows the conventional mean trend case where there is a gradual large scale change in the local mean and no variation in the local variance. This is the classical trend case addressed in virtually all trend literature. Case (c) presents the hard boundary case with two independent sub-domains (s1) and (s2) placed one next to the other. The problem is present only in the local mean, notice the local variances are kept as constant. In case (d), a soft transition (s2) between sub-domains (s1) and (s3) is shown. Notice that in this case the local mean is constant. Usually, this case is considered as stationary, because only variability in the local means is considered as a unique condition for non-stationarity. In case (e) the local means and local variances are assumed as variable with an abrupt change or hard boundary between them. Geologically this case occurs when the two rock types (s1) and (s2) that are assumed to be part of the domain are of independent geologic events, e.g. thin post-mineral dikes (s1) that cross a mineralized host rock (s2). Finally, case (f) shows soft transitions of local means and local variances. Both the local mean and local variance of the sub-domain (s1) slowly increases in the form of (s2) as it reaches sub-domain (s3). Of the cases presented, this can be considered the most realistic. Case (a) is the only one that can be considered as somewhat appropriate to be assumed as multi-Gaussian, however, it is the most uncommon in practice. All other cases are simplistic approximations of reality but fairly practical for modeling after re-scaling local mean and variances. Some authors proposed approaches for dealing with soft boundaries, including McLennan (2007) and Larrondo and Deutsch (2004). For the hard boundary case, there is no other solution but sub-domaining because the two sub-domains involved are independent with no information from one domain contributing in the estimation of the other.

3 Continuous and discrete forms of semivariograms

The variogram can be expressed as a second order moment that measures the variability between two locations separated by a vector $\mathbf{h}$. It is expressed as the variance of the increment of two RVs at locations $\mathbf{u}$ and $\mathbf{u}+\mathbf{h}$, (3) (Journel and Huijbregts 1978).

$$2\gamma(\mathbf{u},\mathbf{u}+\mathbf{h}) = \mathrm{Var}\{Z(\mathbf{u}) - Z(\mathbf{u}+\mathbf{h})\} \tag{3}$$

Notice that there is no restriction about the mean or the variance of the two RVs, and that it does not depend on first or second order stationarity of the RF. Two types of variograms can be obtained, the non-centered (4) and the centered (5) (Gneiting et al. 2001).

$$2\gamma_{NC}(\mathbf{h}) = E\left\{[Z(\mathbf{u}) - Z(\mathbf{u}+\mathbf{h})]^2\right\} \tag{4}$$

$$\begin{aligned} 2\gamma_C(\mathbf{h}) &= \mathrm{Var}\{Z(\mathbf{u}) - Z(\mathbf{u}+\mathbf{h})\} \\ &= E\left\{[Z(\mathbf{u}) - Z(\mathbf{u}+\mathbf{h})]^2\right\} \\ &\quad - [E\{Z(\mathbf{u}) - Z(\mathbf{u}+\mathbf{h})\}]^2 \\ &= 2\gamma_{NC}(\mathbf{h}) - [E\{Z(\mathbf{u}) - Z(\mathbf{u}+\mathbf{h})\}]^2 \end{aligned} \tag{5}$$

Notice in the absence of a drift, both the centered and non-centered variograms are equal. Assuming a SRF, the semivariogram can be linked to the covariance in the form $C(\mathbf{h}) = C(0) - \gamma(\mathbf{h})$. Some semivariograms called unbounded do not have covariance counterparts, such as the power model (Goovaerts 1997; Deutsch 2002). Historically, the reason why geostatisticians preferred the use of the semivariogram over covariance is because the former does not require the previous knowledge of the mean of the RVs for the stationary case (Deutsch and Journel 1997).

In Gneiting et al. (2001), the influence of a trend in the mean in a quadratic form can be filtered using the centered semivariogram (6).

$$\gamma_{NC}(\mathbf{h}) = Q(\mathbf{h}) + \gamma_C(\mathbf{h}) \tag{6}$$

where $Q(\mathbf{h}) = \sum_{i=1}^{d} a_i h_i^2$, $\mathbf{h} = [h_1, \ldots, h_d]^T \in \mathbf{R}^n$, d is the dimension of the Euclidean space, $a_i \geq 0$ for $i = 1, \ldots, d$, and the subscripts C and NC denote centered and non-centered, respectively.

The mean trend does not have any impact in the variability of the realizations of a RV, that is, $\mathrm{Var}\{Z(\mathbf{u})\} = \mathrm{Var}\{R(\mathbf{u}) + m(\mathbf{u})\} = \mathrm{Var}\{R(\mathbf{u})\}$. Recall the mean trend component $m(\mathbf{u})$ at location $\mathbf{u}$ is a single value. However, when considering a regionalized variable sampled over a domain the mean trend inflates the variability, since its effect is additive. Consider a realization z is drawn over a finite domain from an IRF Z, the variance of z is expressed as (7).

$$\sigma_z^2 = \sigma_r^2 + 2C(r, m) + \sigma_m^2 \tag{7}$$

where σ_z^2 is the variance of the sampled values z in the domain, σ_r^2 is the variance of the residuals r in the domain after removing the mean trend in the form (1), σ_m^2 is the variance of the mean trend component in the domain, and $C(r, m)$ the covariance between the residuals r and the mean trend values m at the locations of z in the domain.

In the case where the z values are not influenced by any mean trend, that is, $m_i = c$, then, both terms σ_m^2 and $2C(r, m)$ in (7) are zero, hence only the term σ_r^2 contributes to σ_z^2. This can be considered as the stationary case. Notice in expression (7) there is no requirement that m is a smooth representation of the large scale variability of z in the domain. Both the variability of m and its relationship with r contribute to the variance of z, as shown in (7). Likely, the term $2C(r, m)$ would be expected to be zero since there is no apparent relationship between r and m; therefore, the contributions to the variance of z should come from the variability of r and m in the domain. Consider a scaling factor, $s \in [-1, 1]$, is used to get m in the form $m = s \times r$. The sign of the scaling factor s defines the sign of $C(r, m)$, therefore, σ_z^2 becomes a function of s for this example. For any positive s the variability of z increases as a result of σ_m^2, σ_r^2 and $C(r, m)$, on the other hand, for any negative s as s tends to -1, m will tend to cancel to r and the values of z will tend to zero, hence σ_z^2 tends to decrease. Both σ_m^2 and σ_r^2 contributes to σ_z^2 but $C(r, m)$ reduces it. A relationship between r and m exists when m shares some patterns with r, for the presented example it is the scaling factor s.

However, trends are not noisy structures as presented in the previous example. They are present as large pattern smooth structures in the domain. One of the reasons why the random values r would have a relationship with a trend m of that nature is that m has not been completely removed from z and the residual r is contaminated with some part of m, in the form $m = m' + m''$, where the residual is $r + m'$. The relationship between m' and m'' makes $C(r + m', m'')$ be different from zero. The other reason is due to the non-stationary nature of z; since particular local structural patterns are inherent of the natural process that generated z. In this document r is still considered as a realization of a SRF. The trend contamination is addressed in the following example. Consider a 1D unconditionally simulated dataset of 1,000 regularly spaced data points, separated by 1 unit of distance (uod) (see Fig. 2). A spherical semivariogram model of range of 20uod (8) was used for the simulation.

$$\gamma(\mathbf{h}) = Sph_{20}(\mathbf{h}) \tag{8}$$

Two linear trends are added to the unconditional simulated values (see Fig. 3). The first case is a linear trend with positive slope (see Fig. 3a, b) and the second case is a linear trend with negative slope (see Fig. 3c, d). The correlation coefficients between the unconditional realizations and the trends are 0.104 and −0.104 respectively for the positive and negative slope trends. These values of correlation coefficient make the variances of the combined values z vary from 3.39 for the positive slope trend to 2.78 for the negative slope trend. The variance of the unconditional simulated values σ_r^2 and the

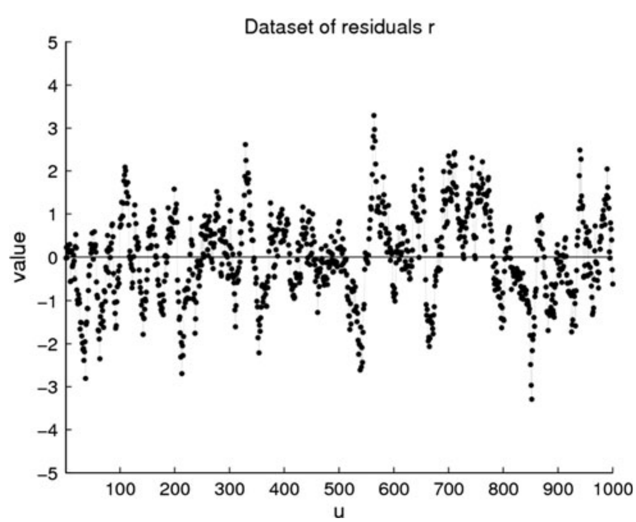


Fig. 2 Unconditional simulated realization of 1,000 data points regularly spaced each 1uod

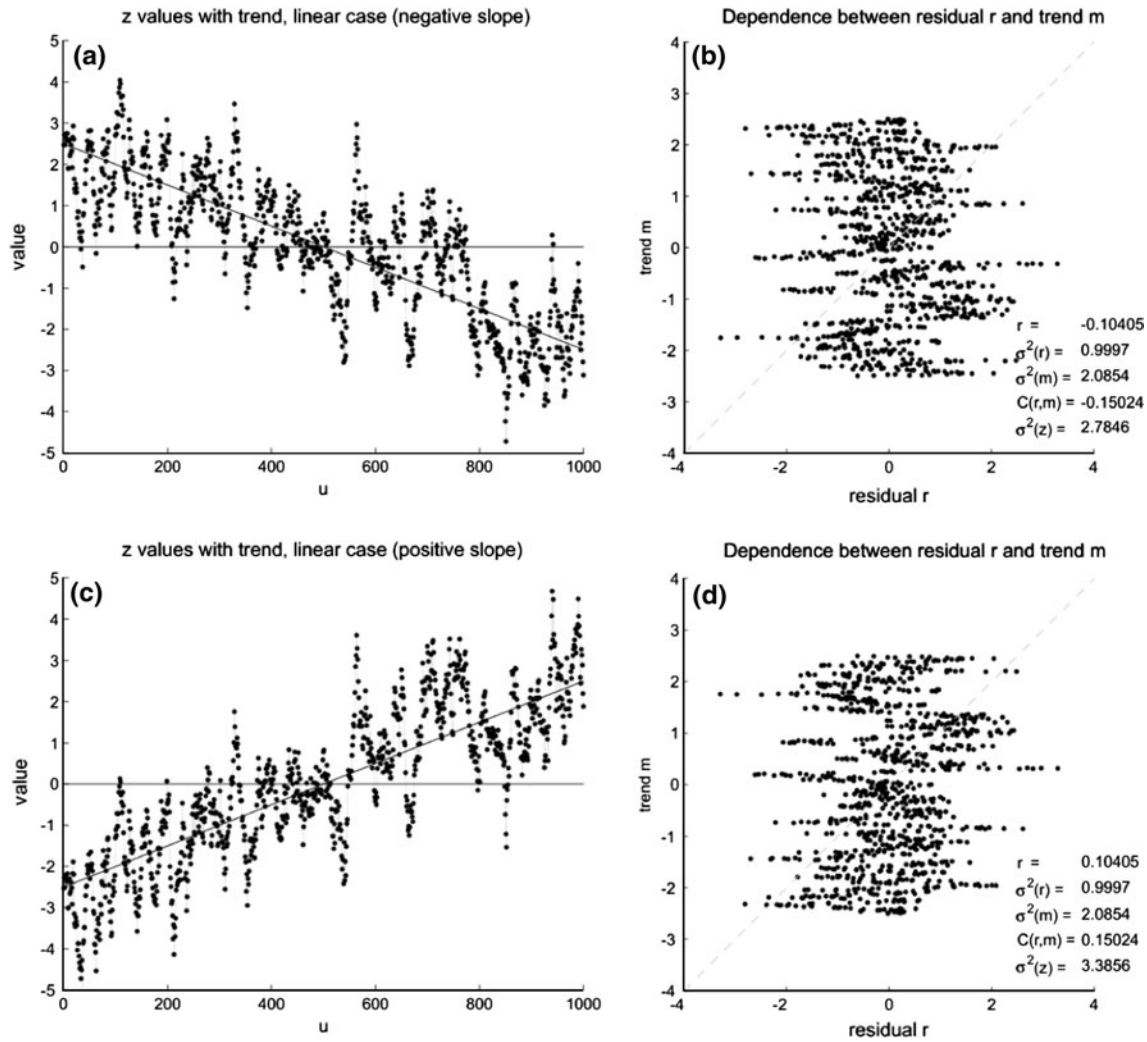


Fig. 3 Two linear trend cases of negative slope (**a**) and positive slope (**c**) added to unconditional simulated realizations and their respective scatter plots between the unconditional realizations and the trend values (**c**, **d**)

variance of the trends σ_m^2 are similar for both cases, only the covariances between the unconditional realization and the trends are different. According to expression (7) these covariances participate in the calculation of σ_z^2 by adding $2C(r, m)$, the values of these terms are 0.30 and -0.30 for the positive and negative slope trend cases and cause the gap between the σ_z^2 values.

For the exercise, the MATLAB detrend tool is used to remove any possible existing mean trend in the unconditional realization r (see Fig. 4a). The new residuals are compared to the previous trend cases in order to verify any relationship between them (see Fig. 4b) and the resulting correlation coefficient is virtually zero. The trend obtained from the unconditional realizations is what initially produced a positive covariance between the unconditional realizations and the first trend case, because both trends have positive slopes. Conversely, for the second trend case where the sign of both trends is different, the covariance between them is negative. The de-trended random variability of the residuals does not have any relationship with any of the trend cases presented in this example and the variance of z, σ_z^2, is the result of the sum of the variance of the de-trended random variability, σ_r^2, and the variance of the trend, σ_m^2. In practice it may be very difficult to remove completely the trend from the z values. However, the present document proposes an approach to identify and quantify the mean and variance trends in the z values.

In conventional geostatistics, the experimental semivariogram is calculated by assuming the RVs belong to a SRF, that is, from the centered semivariogram expression (4). In practice, the calculation is based on the realization data pairs, $\left(z(\mathbf{u}_i), z\left(\mathbf{u}_i + \mathbf{h}_j\right)\right)$, found at the two extremes of each particular separation vector, $\mathbf{h}_j$ (9). This is often referred to as the method-of-moments approach (Matheron 1962). However, the reality is that it is very difficult to find a dataset where data points are separated exactly by $\mathbf{h}_j$. For

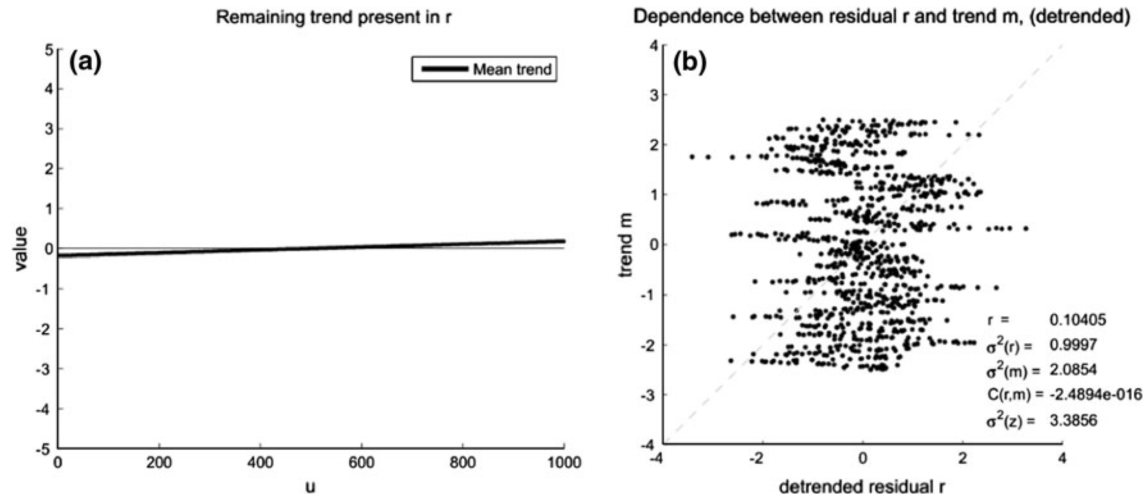


Fig. 4 Linear mean trend present in the unconditional realization r (**a**) and scatter plot between de-trended residual and the positive slope linear trend (**b**)

dealing with this problem, angular and distance tolerances are used to approximate the experimental semivariogram (Deutsch and Journel 1997; Deutsch 2002). The tolerances define a n-dimensional region for each $\mathbf{h}_j$ for a domain in $\mathbf{R}^n$ in order to capture a representative amount of experimental semivariogram pairs $\left(\mathbf{h},\ 0.5[z(\mathbf{u}_i) - z(\mathbf{u}_i + \mathbf{h})]^2\right)$ from a cloud semivariogram.

$$\hat{\gamma}(\mathbf{h}) = \frac{1}{2N(\mathbf{h})}\sum_{i=1}^{N(\mathbf{h})}[z(\mathbf{u}_i) - z(\mathbf{u}_i + \mathbf{h})]^2 \tag{9}$$

4 Impact of mean and variance trends in the semivariogram

During the calculation of the experimental semivariogram (9) the available dataset z, is split in two parts. The first part corresponds to the sub-group at the head of the separation $\mathbf{h}$ vector, $z_{\mathbf{u}}$, and the second part to the sub-group at the tail of the separation vector, $z_{\mathbf{u+h}}$. When the length of the separation vector is zero, both sub-groups consist of all the conditioning data, $z_{\mathbf{u}} = z_{\mathbf{u+h}} = z$. For lengths of the separation vector smaller than half of the size of the domain both the sub-groups at the head and at the tail of the separation vector may share part of the available dataset. Since the domain is finite, the increment in the length of the separation vector is usually accompanied by a reduction in data pairs to calculate the semivariogram. Ideally, under a decision of second order stationarity, the two sub-groups are expected to have the same experimental mean ($m_{\mathbf{u}} \approx m_{\mathbf{u+h}}$) and variance ($\sigma^2_{\mathbf{u}} \approx \sigma^2_{\mathbf{u+h}}$).

The influences of the means and variances of the two sub-groups at the two extremes of the separation vector $\mathbf{h}$ can be obtained by expanding expression (9) and adding the local means of the two sub-groups. Notice in expression (9) the mean trend is assumed to be removed, implying that the second component $0.5[m_{\mathbf{u}} - m_{\mathbf{u+h}}]^2$ should be zero; it should not modify the experimental semivariogram expression if it is calculated in a stationary environment.

$$\begin{aligned}\hat{\gamma}(\mathbf{h}) &= \frac{1}{2N(\mathbf{h})}\sum_{i=1}^{N(\mathbf{h})}\left[(z(\mathbf{u}_i))^2 - 2z(\mathbf{u}_i)z(\mathbf{u}_i+\mathbf{h}) + (z(\mathbf{u}_i+\mathbf{h}))^2\right] \\ &= \frac{1}{2N(\mathbf{h})}\sum_{i=1}^{N(\mathbf{h})}\left[(z(\mathbf{u}_i))^2 + (z(\mathbf{u}_i+\mathbf{h}))^2\right] \\ &\quad - \frac{1}{N(\mathbf{h})}\sum_{i=1}^{N(\mathbf{h})}[z(\mathbf{u}_i)z(\mathbf{u}_i+\mathbf{h})] = \frac{1}{2}\left[\sigma^2_{\mathbf{u}} + \sigma^2_{\mathbf{u+h}}\right] \\ &\quad + \underbrace{\frac{1}{2}[m_{\mathbf{u}} - m_{\mathbf{u+h}}]^2}_{\text{Mean trend component}} - C(\mathbf{h})\end{aligned} \tag{10}$$

Assuming stationarity, the semivariogram is linked to the covariance by $\gamma(\mathbf{h}) = C(0) - C(\mathbf{h})$; a comparison of this expression with (10) shows that the global variance of the domain, assuming the available dataset is fully representative of the domain, is $\sigma^2_z = 0.5(\sigma^2_{\mathbf{u}} + \sigma^2_{\mathbf{u+h}}) + 0.5(m_{\mathbf{u}} - m_{\mathbf{u+h}})^2$. Recall the mean trend component $0.5(m_{\mathbf{u}} - m_{\mathbf{u+h}})^2$ is not part of the global variance, because the term $-0.5(m_{\mathbf{u}} - m_{\mathbf{u+h}})^2$ that cancels the influence of the mean trend component was removed from the experimental semivariogram expression in (9). That is, if the discrete form of the centered semivariogram (5) is used instead of the stationary non-centered semivariogram (4) this mean trend component is cancelled out in (10). If the mean is stationary or the mean trend is removed from the domain, then the variance of the domain is expressed as the average of the respective variances of the two sub-groups, that is, $\sigma_z^2 = 0.5(\sigma_{\mathbf{u}}^2 + \sigma_{\mathbf{u+h}}^2)$. The presence of a mean trend component (10) makes the semivariogram of the dataset increase above the variance of the domain. This is consistent with one of the primary variogram behaviours as documented in Gringarten and Deutsch (2001).

The global variance $0.5(\sigma_{\mathbf{u}}^2 + \sigma_{\mathbf{u+h}}^2)$ without any influence of mean trends can be expressed as $0.5(\sigma_{\mathbf{u}} - \sigma_{\mathbf{u+h}})^2 + \sigma_{\mathbf{u}}\sigma_{\mathbf{u+h}}$ in order to account for differences in the variability of the sub-groups as in the mean trend form. The differences in the variances of $z_{\mathbf{u}}$ and $z_{\mathbf{u+h}}$ are already accounted in the global variance component; therefore, the trend in the variance does not make the experimental semivariogram increase above the sill. Hence, from expression (10) the semivariogram can be re-written as a function of the differences of the standard deviations and difference of the means of $z_{\mathbf{u}}$ and $z_{\mathbf{u+h}}$ (11).

$$\hat{\gamma}(\mathbf{h}) = \underbrace{\frac{1}{2}[\sigma_{\mathbf{u}} - \sigma_{\mathbf{u+h}}]^2}_{\text{Variance trend component}} + \underbrace{\frac{1}{2}[m_{\mathbf{u}} - m_{\mathbf{u+h}}]^2}_{\text{mean trend component}} + \underbrace{\sigma_{\mathbf{u}}\sigma_{\mathbf{u+h}} - C(\mathbf{h})}_{\text{stationary component}} \quad [11]$$

Expression (11) can be re-written so that the correlation coefficient is introduced into the experimental semivariogram expression (12).

$$\hat{\gamma}(\mathbf{h}) = \frac{1}{2}[\sigma_{\mathbf{u}} - \sigma_{\mathbf{u+h}}]^2 + \frac{1}{2}[m_{\mathbf{u}} - m_{\mathbf{u+h}}]^2 + \sigma_{\mathbf{u}}\sigma_{\mathbf{u+h}}(1 - \rho(\mathbf{h})) \quad (12)$$

From expression (11) the experimental semivariogram can be separated into four terms: (a) Half of the squared difference of the standard deviations of the two sub-groups, $0.5[\sigma_{\mathbf{u}} - \sigma_{\mathbf{u+h}}]^2$; (b) half of the squared difference of the means of the two sub-groups, $0.5[m_{\mathbf{u}} - m_{\mathbf{u+h}}]^2$; (c) the product of the two standard deviations of the two sub-groups, $\sigma_{\mathbf{u}}\sigma_{\mathbf{u+h}}$; and (d) the covariance between the two sub-groups, $C(\mathbf{h})$. Notice when the means and variances of the two sub-groups are similar, i.e. $\sigma_{\mathbf{u}} \approx \sigma_{\mathbf{u+h}} \approx \sigma$ and $m_{\mathbf{u}} \approx m_{\mathbf{u+h}} \approx m$, the experimental semivariogram expression (11) relies only on components (c) and (d) which is very similar to the stationary form of the semivariogram, $\hat{\gamma}(\mathbf{h}) = \sigma^2 - C(h)$.

It is often presented that when the experimental semivariogram is above the variance of the dataset or sill, then the correlation between the two sub-groups separated by **h** is negative (Gringarten and Deutsch 2001; Deutsch 2002; Leuangthong and Deutsch 2004). However, linear mean trends as presented in Fig. 3 can cause the experimental semivariogram rise above the sill, while still maintaining a positive correlation between the two sub-groups. The influence of mean trends and the negative correlation case between sub-groups separated by **h** are discussed further in this document.

5 Method-of-moments and trends in the experimental semivariogram

Under stationary conditions for all the **h**-scatter plots of the available dataset, the means and variances of the marginal distributions are expected to be very similar. Systematic differences in them as a result of increasing the length of the separation vector would imply a presence of mean or variance trends in the domain which can be captured by the experimental semivariogram (11). In this section, the unconditional realization of 1,000 regularly spaced simulated data points using the semivariogram model (8) is used. To this dataset, three trend cases are added (Fig. 5):

(1) A linear trend in the form $y = ax + b$ with a negative slope a along the entire domain. This case accounts for a large variability in the local means.
(2) A symmetrically concave-shaped trend case. This mean trend is presented in order to show a special case and how this approach accounts for this type of symmetric trend.
(3) A variance trend with no presence of mean trend. For this, the variances of the two halves of the domain are re-scaled.

The experimental semivariograms are calculated using expression (11) in order to quantify the impact of the mean and variance trends in the domain. The semivariogram plots for each case are calculated within a range of one half the size of the domain and the contributions of each component of the experimental semivariogram are color coded in gray scale for visualization (see Fig. 6).

For the stationary case (Fig. 6a) almost all lags of the experimental semivariogram are free of mean and variance trends. Notice the mean trend identified in the initial dataset in the previous section has been also identified by this approach as a small region as well as small presence of a variance trend. The experimental semivariogram of the initial dataset combined with the linear mean trend case (Fig. 6b) shows the mean trend component pushes the stationary component upward; making it possible for the experimental semivariogram to rise above the sill. For this type of linear trend, the mean trend component increases monotonically. The symmetric case of a parabolic mean trend (Fig. 5d) shows that the mean trend is not recognized in the experimental semivariogram (Fig. 6c). The stationary component of the experimental semivariogram is above the sill when negative correlations between the sub-groups are caused by the mean trend. Because of the symmetric shape of this trend, the mean trend component is cancelled

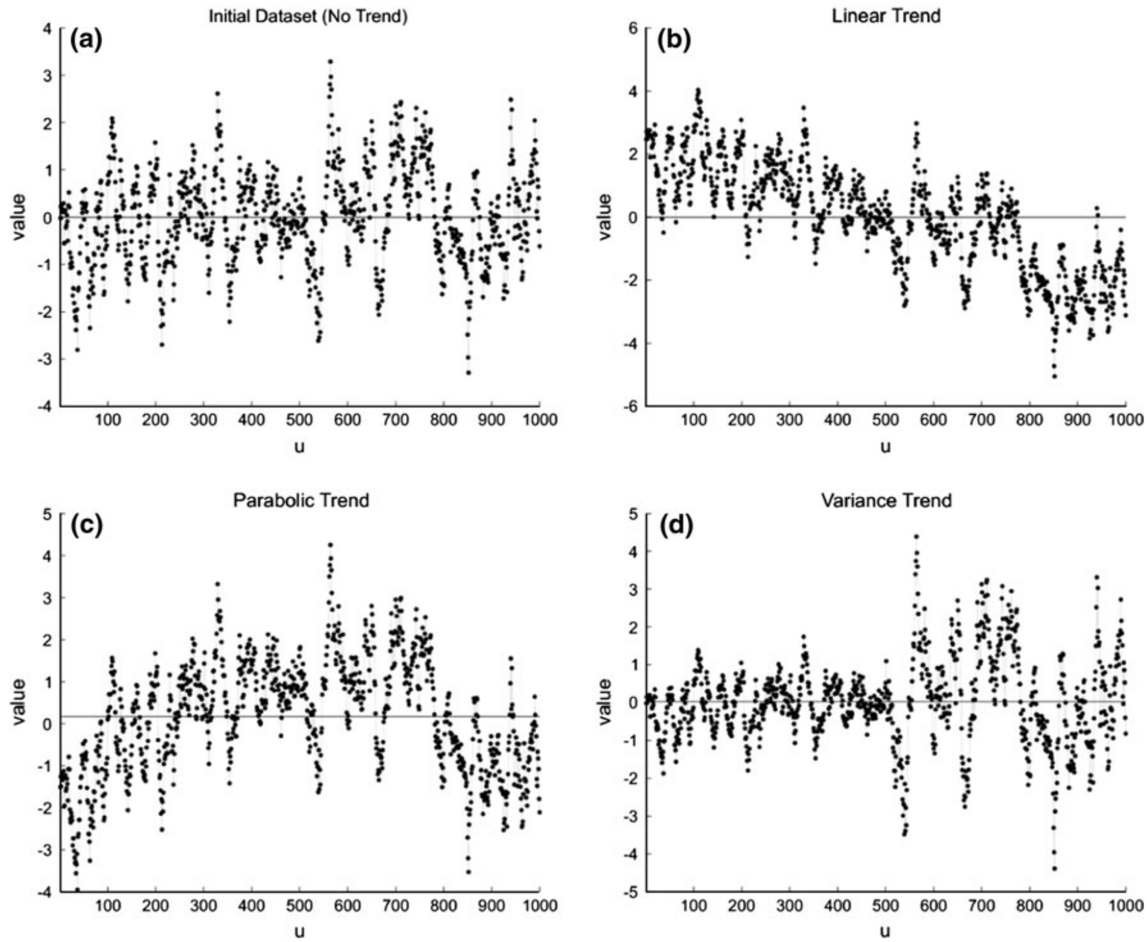


Fig. 5 Initial dataset (**a**) influenced by linear mean trend (**b**), symmetric mean trend (**c**) and local variability in variances (**d**)

out in the experimental semivariogram and is considered to be part of the random fluctuation of the residuals. This condition is characteristic of this type of symmetric mean trend. The variance trend case (Fig. 5d) can be identified in the experimental semivariogram as a sub-region in the stationary component (Fig. 6d) and it does not make the experimental semivariogram rise above the current sill. However, the sill of the semivariogram is not representative of the domain. It would be incorrect to use this semivariogram for modeling.

In the first case (Fig. 6a) there is no influence of mean or variance trends and the experimental semivariogram reaches the variance of the domain and is relatively constant with some ergodic fluctuations beyond the semivariogram range. However, the mean trend that was earlier indentified in this dataset is assumed to be negligible herein. The light gray region represents the stationary component of the experimental semivariogram, $\sigma_{\mathbf{u}}\sigma_{\mathbf{u}+\mathbf{h}} - C(\mathbf{h})$, in (11). This is considered as the ideal case of a stationary domain. At each lag separation, **h**, the **h**-scatter plots show that the cloud of data pairs are centered along the 45° bisector. This implies the local means and variances of the sub-groups at **u** and **u** + **h** are similar (see Fig. 7).

In the second case (Fig. 6b), the linear mean trend makes the experimental semivariogram increase and at a certain point it becomes larger than the variance of the domain. Notice the stationary part behaves similar to the experimental semivariogram of the first case (light gray region), while the mean trend (gray region) is the only source of additional increment in the experimental semivariogram. If the centered semivariogram (5) is calculated the mean trend contribution is cancelled out leaving only the stationary region. The differences in the local means is what makes the cloud of data pairs in the **h**-scatter plots to be non-centered, increasing the distances of the data pairs from the 45° bisector as the lag distance increases. Hence the experimental semivariogram may be above the variance of the domain while the correlation coefficient of the **h**-scatter plot is still positive (see Fig. 8).

The third trend scenario (see Fig. 6c) results in a special case where the contribution of the mean trend component

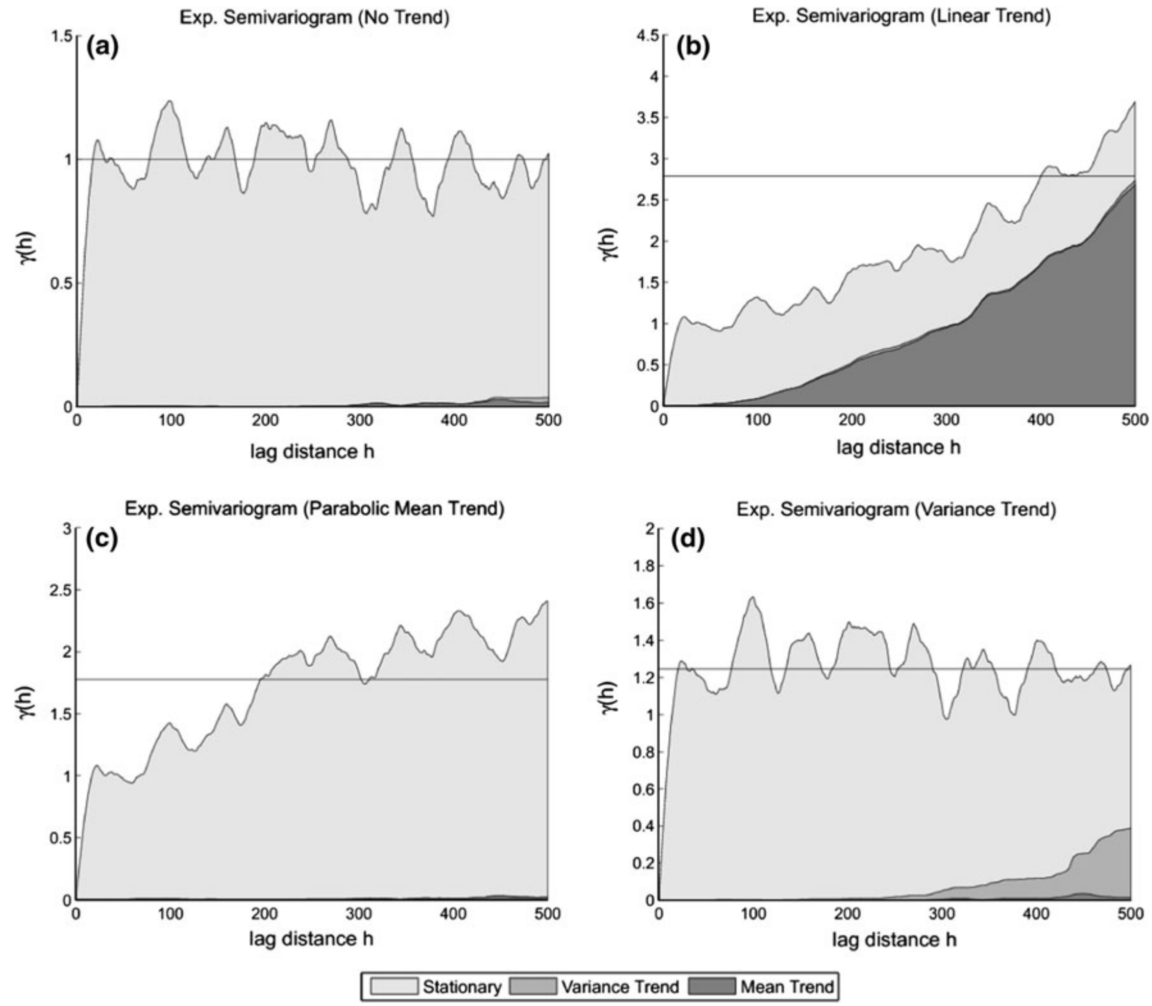
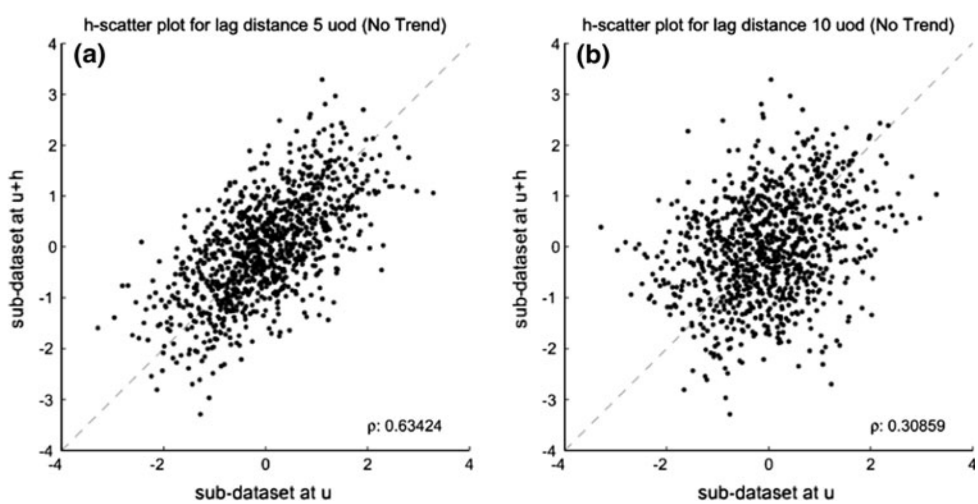


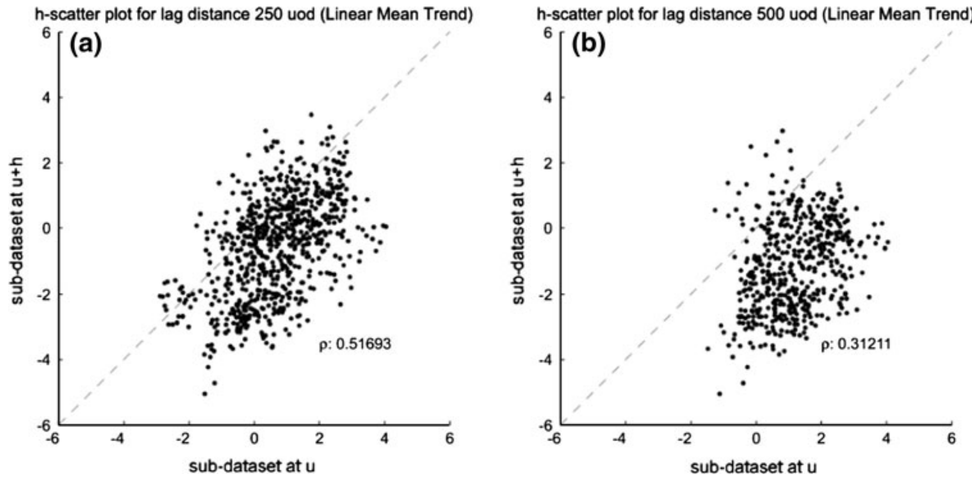
Fig. 6 Experimental variograms for initial dataset (unconditional simulated realization) (**a**) and influenced by linear mean trend (**b**), symmetric mean trend (**c**) and locally variable variance (**d**)

Fig. 7 **h**-Scatter plots for stationary case for lag distances 5 uod (**a**) and 10 uod (**b**)



cannot be seen in the experimental semivariogram plots. Recall that, the mean trend component is captured when differences in the means of the sub-groups appear as the separation distance increases. For this case, the mean trend component in the experimental semivariogram is cancelled, since $m_{\mathbf{u}} \approx m_{\mathbf{u+h}}$, therefore, $m_{\mathbf{u}} - m_{\mathbf{u+h}} \approx 0$, and the

Fig. 8 **h**-Scatter plots for linear mean trend case for lag distances 250 uod (**a**) and 500 uod (**b**)



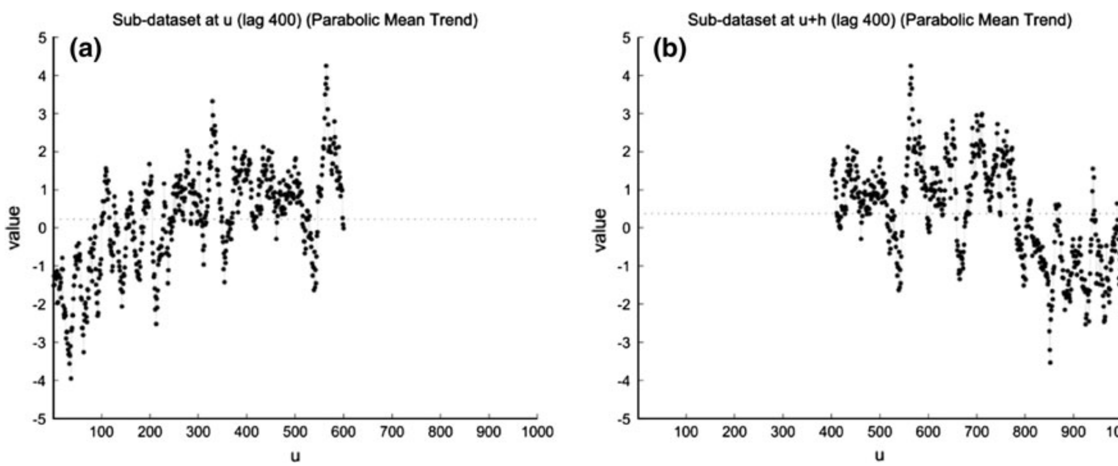


Fig. 9 Sub-groups of the available dataset influenced by a parabolic mean trend at the head (**a**) and tail (**b**) of the separation vector **h** for a separation distance of 400 uod

trend curve is considered as part of random fluctuation. In such case, the mean trend is mirrored when calculating the experimental semivariogram (see Fig. 9). As the length of the separation vector increases the covariance between the two sub-groups $z_{\mathbf{u}}$ and $z_{\mathbf{u+h}}$ tends to mask the variability of the initial dataset because of the trend component and the covariance becomes negative (see Fig. 10), making the experimental semivariogram increase above the sill. The characteristic that the experimental semivariogram increases above the sill with no apparent contribution of the mean trend component is a signature of this type of mean trend.

In the fourth case, the experimental semivariogram does not show any tendency to grow above the sill. This is because the trend in the variance does not contribute to the semivariogram (see Fig. 6d). In the **h**-scatter plots the variance trend increases with the difference in the variances of the marginal distributions of the two sub-groups at the two extremes of the separation vector **h** (see Fig. 11). Notice the differences in the variances of the two sub-groups shrink the cloud of data pairs in the horizontal direction because the first half of the dataset is the one with smaller local variance (see Fig. 5d). If the variance trend goes in the opposite direction, the cloud of data pairs will tend to shrink vertically.

6 Discussion

Determining the influence of the local mean and/or variance trends on the semivariogram requires a representative sampling of the domain. In presence of large unsampled regions in the domain or blank spots, this approach may lead to misinterpretation of the results. Even in instances where the intention is not to identify presence of trends, the calculated experimental semivariograms is unreliable under these conditions.

Depending on the scale of the observation, the domain may present an apparent trend (see Fig. 12). Some

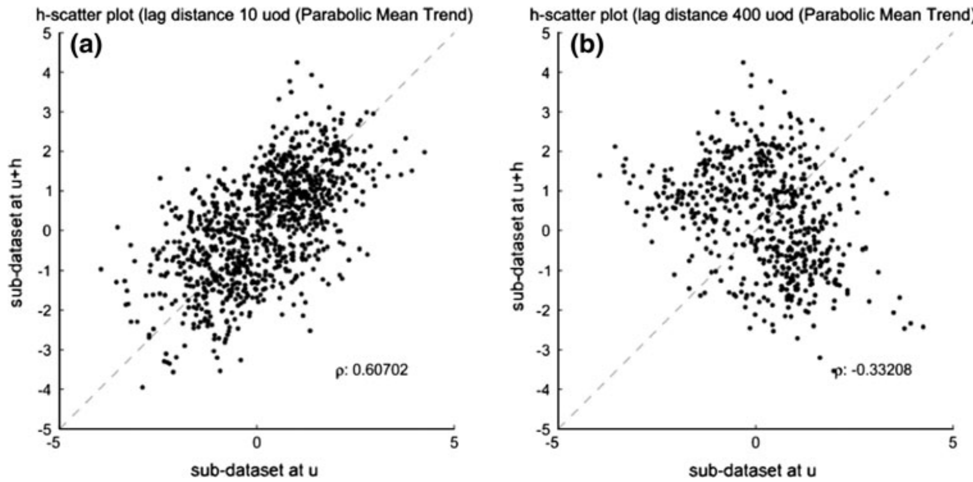


Fig. 10 **h**-Scatter plots for the parabolic shaped trend case for lag distances 10 uod (**a**) and 400 uod (**b**)

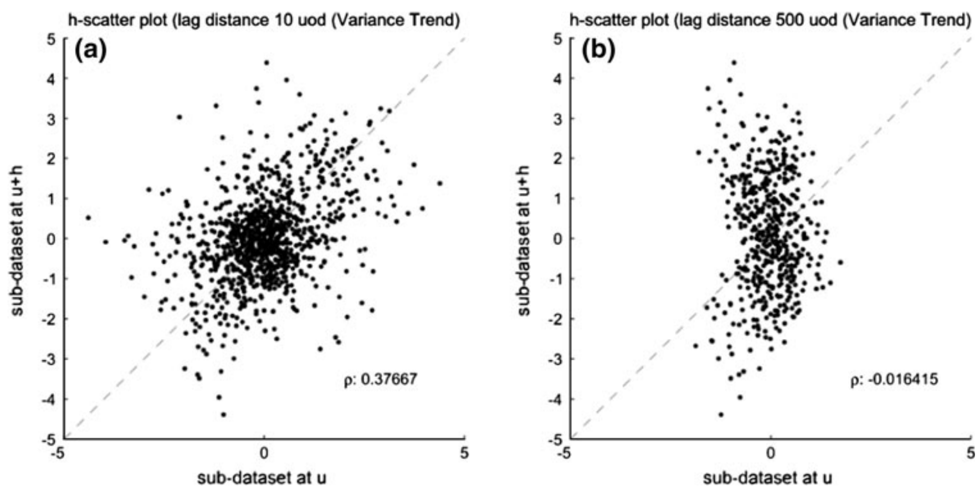


Fig. 11 **h**-Scatter plots for the variance trend case for lag distances 10 uod (**a**) and 500 uod (**b**)

techniques like universal kriging and ordinary kriging consider a semivariogram model fitted from the experimental semivariogram of the dataset with trend. The problem of assuming stationarity of the partial dataset with apparent mean trend (Fig. 12c) is that the semivariogram of the large scale stationary process (Fig. 12b) is not accessible. The semivariogram with apparent mean trend tends to inflate the global variance as well as to exaggerate the spatial continuity (Fig. 12d). From the partial dataset, without the knowledge of the features of the complete dataset, it is not possible to determine whether the trend is apparent or representative. Therefore, it is recommended to remove any presence of mean and/or variance trend in the dataset prior to building a geostatistical model because of the possible consequences.

Although the examples given in this paper are one dimensional for ease of illustration and dissection of the trend sources, there is no limitation to applying this decomposition to two or three dimensions. Since semivariograms are directional in nature, a trend is often apparent in one direction and not the other. Figure 13 shows an example of a semivariogram calculated for a two-dimensional topographic dataset, where a mean trend is easily detected in the north–south direction and an apparent zonal anisotropy is visible in the east–west direction. This example shows the source of the trend is attributed to the mean component with negligible variance contribution.

Even in presence of a densely sampled data over a domain, mean trends should be removed prior to modelling. Recall that the semivariogram, when influenced by mean trends, tends to exaggerate the spatial continuity and inflate the conditional variances. It results in an estimated model that may be much smoother than it should be and the uncertainty inflated. This is perhaps difficult to discern locally in those regions with lots of samples, but it should be more apparent in other regions with sparse data. A semivariogram influenced by a trend should not be used as an input of a geostatistical modeling technique in any case. Therefore, even in presence of abundant data, the modeler should still take care in considering the impact of the trend.

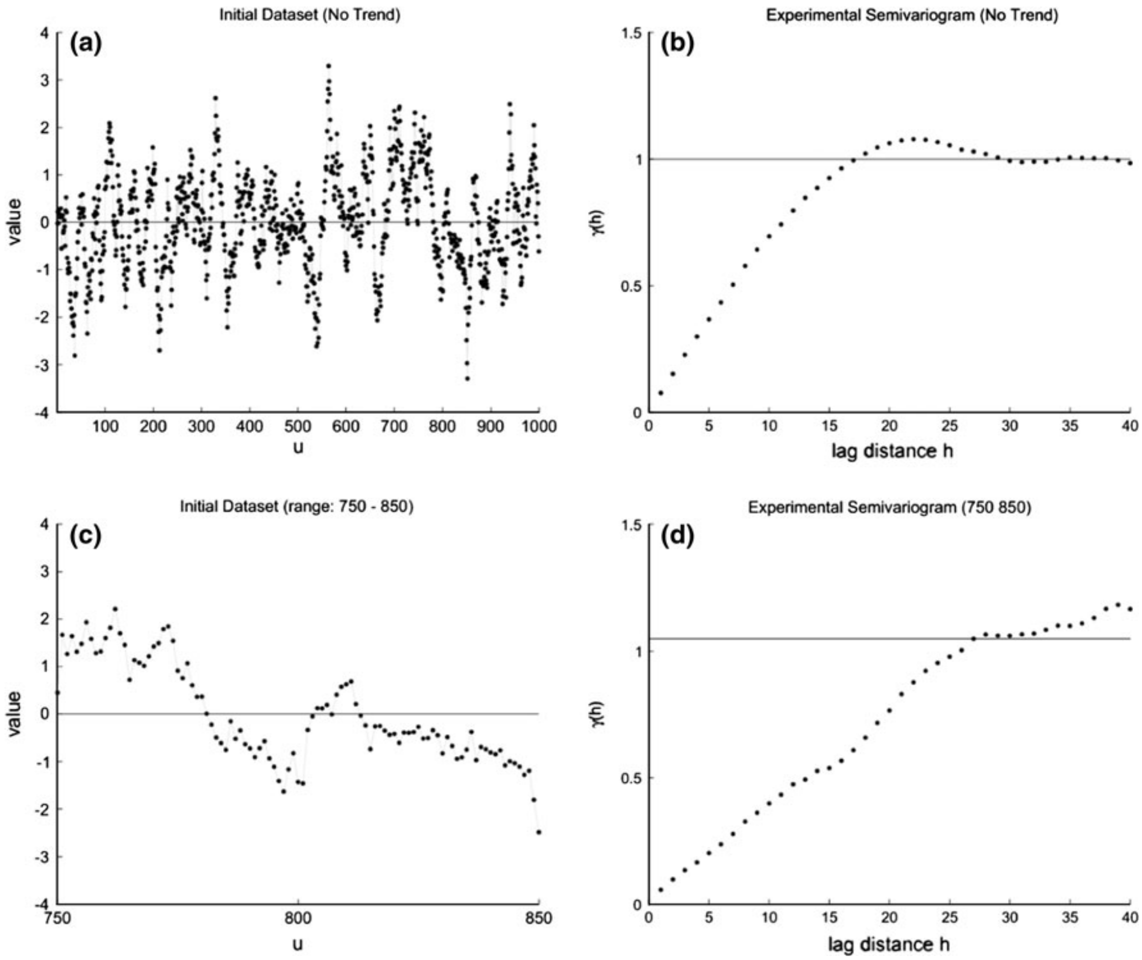


Fig. 12 Unconditional simulated dataset (**a**) and its corresponding experimental semivariogram without influence of any trend (**b**), a segment of the unconditional simulated dataset of 100 data points with apparent mean trend (**c**) and its experimental semivariogram (**d**)

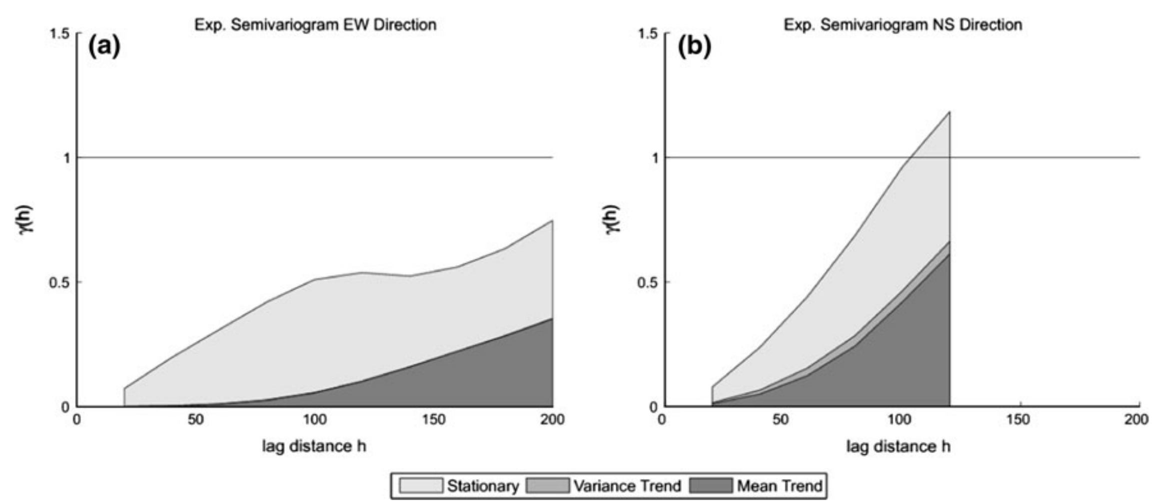


Fig. 13 Decomposed experimental semivariogram from topographic samples in normal score units for south–north (**a**) and east–west (**b**) directions

7 Conclusions

Non-stationary features such as mean and variance trends of the dataset can be captured by analyzing the experimental semivariogram. Differences in the local means and local variances are identified by comparing the sub-groups of datasets at the two extremes of the separation vector. It is important to keep in mind the semivariogram is a two point statistic and as such it may not adequately capture complex trend features in the RF such as the concave/convex symmetric mean trend cases. However, this type of complex mean trend structures can be captured with the use of generalized covariances (Chilès and Delfiner 1999), where the spatial variability of the domain is verified by taking configurations with more than two points as in the semivariogram case.

The decision to accept or reject a certain domain prior to geostatistical modeling can be made by using the proposed approach for identifying trends in the domain and is based on expert judgement. Accepting a domain implies that mean and variance trends do not present a problem, and avoids possible issues like global variance inflation or artificial increases in the variogram range in the final result. If the domain is rejected, additional pre-processing such as sub-domaining and/or de-trending of the domain are necessary until mean and/or variance trends do not represent a problem in the domain. Even when the mean and variance trends are removed from a dataset, it cannot be considered as stationary yet. There is one additional condition that should be verified, which is the stationarity of the spatial covariance. Moreover, the performance of any technique proposed for dealing with mean and/or variance trends can be tested by this form of the experimental semivariogram.

The decomposition of the experimental semivariogram does not require any additional information to that of conventional semivariogram calculation. It permits quantification of the sources that contribute to a trend, thereby allowing for more suitable detrending approaches to be considered for resource modeling.

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