Breccia Pipe Prediction: a new approach using non-stationary covariances

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Abstract

In this paper, we are interested in the prediction of the breccia pipe elevation named "Braden" of the El Teniente mine in Chile. The problem is tackled by developing a new geostatistical approach based on non-stationary covariances. The proposed method offers an integrated treatment of all aspects of non-stationarity: mean, variance and spatial continuity. The estimation of non-stationary parameters is free distribution and carried out under the local stationarity assumption. The resulting estimated non-stationary parameters are naturally integrated into a kriging procedure or conditional simulations. The proposed approach has revealed an increased prediction accuracy when compared to the stationary one and demonstrated the ability to extract the underlying non-stationarity.

1 Introduction

A canonical problem in the geosciences is the prediction of a physical quantity over the whole region of interest from a finite set of irregular spaced data. This problem involves modeling and estimating the underlying spatial dependence structure of the observed data. Commonly, this is accomplished through statistical tools such as the variogram or covariogram computed on the whole domain of interest, under the stationarity assumption. However, in practice the stationarity assumption can be doubtful due to many factors, including specific landscape and topographic features of the region of interest or other localized effects. These local influences can be reflected computing local variograms, whose characteristics may vary across the domain of study. In such cases, carry out predictions based on a stationary approach could produce less accurate predictions, including an incorrect assessment of the estimation error (Stein, 1999).

Several approaches have been proposed for modeling and estimating non-stationary dependence structure (see Guttorp and Schmidt (2013), for a brief review). One of the most interesting is the explicit non-stationary covariances class proposed by Paciorek and Schervish (2006). However, the parameter estimation of these latter remains a crucial problem. In this work, we develop a procedure of estimating parameters that govern this class of closed-form non-stationary covariances under a single realization and local stationarity framework, through a step by step approach. First, we compute local variograms by a non-parametric kernel estimator. Then, it is used in a weighted local least squares procedure for estimating the parameters at a reduced set of representative points referred to as anchor points. Finally, a kernel smoothing method is used to interpolate the parameters at any location of interest. Then, the estimated non-stationary parameters are integrated naturally into a kriging procedure or conditional simulations.

As a motivating example in this work we consider the prediction of the breccia pipe elevation named "Braden" of the El Teniente mine in Chile. This latter is one of the largest known porphyry-copper ore bodies. The pipe is poorly mineralized and surrounded by different kinds of mineralized geological units. Knowing the exact location of the pipe surface is important, as it constitutes the internal limit of the deposit. Previous approaches have been applied on this dataset by Séguert and Celhay (2013).
The paper is structured as follows: the model formulation is described in Section 2. In Section 3, the statistical inference is detailed. Spatial predictions and conditional simulations are presented in Section 4. In Section 5, the proposed approach is applied on the breccia pipe datasets. Section 6 is a concluding remarks.

2 Model Formulation

Let \( Y = \{ Y(x) : x \in G \subset \mathbb{R}^p, p \geq 1 \} \) be a random field defined on a fixed continuous domain of interest \( G \) of the Euclidean space \( \mathbb{R}^p \) and reflecting the underlying studied phenomenon. We consider that \( Y \) is governed by the following model:

\[
Y(x) = m(x) + \sigma(x)Z(x), \quad \forall x \in G,
\]

where: \( m : \mathbb{R}^p \to \mathbb{R} \) is an unknown fixed function; \( \sigma : \mathbb{R}^p \to \mathbb{R}^+ \) is an unknown positive fixed function; \( Z \) is a zero-expectation, unit variance random field with correlation function defined by:

\[
R^{NS}(x, y) = \phi_{xy} R^S \left( \sqrt{Q_{xy}(x-y)} \right), \quad \forall (x, y) \in G \times G,
\]

with: \( \phi_{xy} = |\Sigma_x|^{\frac{1}{2}} |\Sigma_y|^{\frac{1}{2}} \left| \Sigma_x + \Sigma_y \right|^{-\frac{1}{2}}, \quad Q_{xy}(h) = h^T \left( \frac{\Sigma_x + \Sigma_y}{2} \right)^{-1} h, \quad \forall h \in \mathbb{R}^p; \)

\( \Sigma : \mathbb{R}^p \to PD_r(\mathbb{R}), x \mapsto \Sigma_x \) is a mapping from \( \mathbb{R}^p \) to \( PD_r(\mathbb{R}) \) the set of real-valued positive definite \( p \)-dimensional square matrices; \( R^S(.) \) is a continuous isotropic stationary correlation function, positive definite on \( \mathbb{R}^p \), for all \( p \in \mathbb{N}^* \).

The expression (2) represents the closed form non-stationary covariances class proposed by Paciorek and Schervish [2006]. The construction of this class is based on a convolution of an orthogonal random measure with a spatially varying random weighting function (see Fouedjio et al. [2014] for more details). We can notice that this class gives non-stationary versions of some well known stationary correlation functions (Gaussian, exponential, Matérn and Cauchy) for a specific choice of \( R^S(.) \). The intuition behind this class is that to each location \( x \) is assigned a local Gaussian kernel matrix \( \Sigma_x \) and the correlation between two locations \( x \) and \( y \) is calculated by averaging between the two local kernels at \( x \) and \( y \). In this way, the local characteristics at both locations influence the correlation of the corresponding target values. Thus, it is possible to account for non-stationarity. It is done by specifying the mapping \( \Sigma(.) \) which models the anisotropy of the correlation function. The resulting kernel matrix \( \Sigma_x \) at each point \( x \) is interpreted as a locally varying geometric anisotropy matrix. It controls the anisotropic behavior of the random field in a small neighborhood around \( x \).

From model defined in (1), the two first moments of the random field \( Y \) is given by:

\[
E(Y(x)) = m(x),
\]

\[
\text{Cov}(Y(x), Y(y)) = \sigma(x)\sigma(y)R^{NS}(x, y) \equiv C^{NS}(x, y).
\]

Then, the non-stationarity of the random field \( Y \) is characterized by the non-stationary parameters \( m(.) \), \( \sigma(.) \) and \( \Sigma(.) \) defined at any location of the region of interest.

3 Statistical Inference

Let \( Y = (Y(s_1), \ldots, Y(s_n))^T \) be a \( (n \times 1) \) vector of observations from a unique realization of the random field \( Y \), associated to known locations \( \{s_1, \ldots, s_n\} \subset G \subset \mathbb{R}^p \). The objective is to use the data \( Y \) to estimate the mean function \( m(.) \), the standard deviation function \( \sigma(.) \) and the correlation function determined by \( \Sigma(.) \). The estimation of these parameters relies on the slightly local stationarity assumption which allows certain simplifications.
3.1 Local Stationarity

The local stationarity assumption [Matheron (1971)] implies that at any location \( x_0 \in G \) there exists a neighborhood \( \mathcal{V}_{x_0} = \{ x \in G, \| x - x_0 \| \leq b \} \) where the random field \( Y \) can be approximated by a stationary random field. Thus, \( \forall (x, y) \in \mathcal{V}_{x_0} \times \mathcal{V}_{x_0}, m(x) \approx m(y) \approx m(x_0) \) and \( C^{NS}(x, y) \approx C^S(x - y; x_0) = C^S(h; x_0), \| h \| \leq b \); where \( C^S(.) \) is a stationary covariance and the limit \( b \) represents the radius of the local stationarity neighborhood \( \mathcal{V}_{x_0} \). In this way, the parameters are assumed to be very smooth functions which vary slowly over the domain. The expectation of the random field \( Y \) being approximately equal to a constant inside the local stationarity neighborhood, the resulting local covariance structure at any location \( x_0 \) is written as follows:

\[
C^S(h; x_0) = \sigma^2(x_0) R^S \left( \sqrt{h^T \Sigma_{x_0}^{-1} h} \right), \| h \| \leq b. \tag{5}
\]

Locally, the non-stationary covariance \( C^{NS}(\cdot, \cdot) \) is thus reduced to an anisotropic stationary one \( C^S(\cdot) \). The anisotropy function \( \Sigma(.) \) is parametrized through the spectral decomposition and then the positive definiteness is guaranteed. Precisely, at any location \( x_0 \in G \), \( \Sigma_{x_0} = \Psi_{x_0} \Lambda_{x_0} \Psi_{x_0}^T \), where \( \Lambda_{x_0} \) is the diagonal matrix of eigenvalues and \( \Psi_{x_0} \) is the eigenvector matrix. We assume working in 2D (\( p = 2 \)) from now and we have:

\[
\Lambda_{x_0} = \begin{pmatrix}
\lambda_1^2(x_0) & 0 \\
0 & \lambda_2^2(x_0)
\end{pmatrix}, \quad \Psi_{x_0} = \begin{pmatrix}
\cos(\psi(x_0)) & \sin(\psi(x_0)) \\
-\sin(\psi(x_0)) & \cos(\psi(x_0))
\end{pmatrix}, \quad \lambda_1(x_0), \lambda_2(x_0) > 0 \quad \text{and} \quad \psi(x_0) \in [0, \pi).
\]

At each point, the square roots of the eigenvalues control the local ranges and the eigenvector matrix specify the local orientations. Thus, the anisotropy function \( \Sigma(.) \) is characterized by the functions \( \lambda_1(\cdot), \lambda_2(\cdot) \) and \( \psi(\cdot) \).

3.2 Local Variogram Kernel Estimator

Under the local stationarity assumption, we define a non-parametric kernel moment estimator of the stationary local variogram at a fixed location \( x_0 \in G \) and lag \( h \in \mathbb{R}^p \), \( \gamma(h; x_0) = \sigma^2(x_0) - C^S(h; x_0), \| h \| \leq b \) as follows:

\[
\hat{\gamma}_a(h; x_0) = \frac{\sum_{V(h)} K^*_s(x_0, s_i) K^*_s(x_0, s_j) |Y(s_i) - Y(s_j)|^2}{2 \sum_{V(h)} K^*_s(x_0, s_i) K^*_s(x_0, s_j)}, \| h \| \leq b, \tag{6}
\]

where the average \( \{ \} \) is taken over \( V(h) = \{ (s_i, s_j) : s_i - s_j = h \} \), the set of all pairs of locations separated by vector \( h \); \( K^*_s(x_0, s_i) = K_s(x_0, s_i)/\sum_{l=1}^n K_s(x_0, s_i) \) are standardized weights; \( K_s(\cdot, \cdot) \) is a non-negative, symmetric kernel on \( \mathbb{R}^p \times \mathbb{R}^p \) with bandwidth parameter \( \epsilon > 0 \).

This moment estimator of the local variogram at any location \( x_0 \in G \) is a kernel weighted local average of squared differences of the regionalized variable. The kernel function is used to smoothly down-weight the squared differences (for each lag interval) according to the distance of these paired values from a target location. We assign to each data pair a weight proportional to the product of the individual weights. Observation pairs near to the target location \( x_0 \) have more influence on the local variogram estimator than those which are distant.

To calculate the non-parametric kernel estimator \( \hat{\gamma}_a \), we choose an isotropic stationary Gaussian kernel: \( K_\epsilon(x, y) \propto \exp\left(-\frac{1}{2\epsilon^2}\|x - y\|^2\right), \forall (x, y) \in G \times G \). The latter has a non-compact support and therefore considers all observations. Thus, the local variogram estimator is not limited only to the local information, distant points are also considered. This avoids artefacts caused by the only use of observations close to the target location. It also reduces instability of the obtained local variogram at regions with low sampling density. Furthermore, it provides a smooth parameter estimate and then is compatible with the quasi-stationarity assumption. The size of the quasi-stationarity neighborhood \( b \), it is set with respect to the bandwidth \( \epsilon \). We take \( b = \sqrt{3} \epsilon \) such that the standard deviation of the isotropic stationary Gaussian kernel matches the isotropic stationary uniform kernel (with compact support).
3.3 Parameter Estimation

The estimation of the parameters vector \( \theta(x_0) = (\sigma(x_0), \lambda_1(x_0), \lambda_2(x_0), \psi(x_0)) \) which characterizes the stationary local variogram \( \gamma(\cdot; x_0) \equiv \gamma(\cdot; \theta(x_0)) \) at a fixed location \( x_0 \) are found via the following minimization problem:

\[
\hat{\theta}(x_0) = \arg \min_{\theta(x_0) \in \Theta} \| w_c(x_0) \odot (\gamma(\theta(x_0)) - \hat{\gamma}_c(x_0)) \| ,
\]

where \( \odot \) is the product term by term; \( \gamma^T(\theta(x_0)) = [\gamma(h_j)]_{j=1}^{J} ; \hat{\gamma}^T_c(x_0) = [\hat{\gamma}_c(h_j; x_0)]_{j=1}^{J} ; \) \( w_c^T(x_0) = [w_c(h_j; x_0)]_{j=1}^{J} ; w_c(h; x_0) = \left[ \sum_{V(h)} K^*_e(x_0, s_i) K^*_e(x_0, s_j) / ||h|| \right]^{1/2} ; \) \{h_j \in \mathbb{R}^p, j=1,\ldots,J\} are given lag vectors; \( \theta(x_0) \in \Theta \) is the vector of unknown parameters and \( \Theta \) is an open parameter space.

Using the estimate of the vector of structural parameters \( \hat{\theta}(x_0) \) obtained in (7), the mean parameter \( m(x_0) \) is estimated explicitly by a local stationary kriging of the mean (Matheron 1971).

For the prediction purpose, one needs to compute the non-stationary parameters \( m(\cdot), \sigma(\cdot) \) and \( \Sigma(\cdot) \) at prediction and observation locations. In practice, it is unnecessary to solve the minimization problem (7) at each target location. Indeed, doing so is computationally intensive and redundant for close locations, since these estimates are highly correlated. To reduce the computational burden, the proposed idea consists in obtaining the parameter estimates only at some reduced set of \( m \ll n \) representative points referred to as anchor points defined over the domain of interest. Then, using the estimates obtained at anchor points, a kernel smoothing method is used to make available estimates at any location of interest. We works with the Nadaraya-Watson kernel smoother which is appropriate and relatively simple. However, other smoothers can be used as well (local polynomials, splines, etc.). The choice of the smoothing bandwidth associated to Nadaraya-Watson kernel smoother is done through the generalized cross-validation criteria (Wand and Jones 1995).

The estimation of the non-stationary parameters depends on the bandwidth parameter \( \epsilon \) used in the computation of the local variogram non-parametric kernel estimator defined in (6). Indeed, the size of the local stationarity neighborhood is expressed in terms of this bandwidth parameter. The data-driven method used to select the bandwidth \( \epsilon \) consists of leaving out one data location and using a form of cross-validation. Because the estimation of the spatial dependence structure is rarely a goal per se but an intermediate step before kriging, we want to choose the bandwidth that gives the best cross-validation mean square error.

4 Prediction

The main purposes of modelling and estimating the spatial dependence structure is to spatially interpolate data and perform conditional simulations. The expected benefit using the closed-form non-stationary covariances class (4) is to obtain spatial predictions and variance estimation errors more realistic than those based on an inadequate stationary covariances.

4.1 Kriging

Let \( C^{NS}(\cdot, \cdot) \) the non-stationary covariance of the random field \( Y \) and \( m(\cdot) \) its mean. Given the vector of observations \( \mathbf{Y} = (Y(s_1), \ldots, Y(s_n))^T \) at \( n \) fixed locations \( s_1, \ldots, s_n \in G \), the point predictor for the unknown value of \( Y \) at unsampled location \( s_0 \in G \) is given by the optimal linear predictor:

\[
\hat{Y}(s_0) = m(s_0) + \sum_{i=1}^{n} \eta_i(s_0) (Y(s_i) - m(s_i)).
\]
The kriging weight vector $\eta = [\eta_i(s_0)]$ and the corresponding kriging variance $Q(s_0)$ are given by:

$$\eta = C^{-1}C_0 \quad \text{et} \quad Q(s_0) = \sigma^2(s_0) - C_0^T C^{-1} C_0. \quad (9)$$

where $C_0 = [C^{NS}(s_i, s_0)]; \quad C = [C^{NS}(s_i, s_j)]$.

### 4.2 Conditional Simulations

Here we assume that the random field $Y$ is Gaussian with mean $m(.)$ and non-stationary covariance structure $C^{NS}(.,.)$. We want to simulate at a large number of locations a Gaussian random field with same mean and covariance, and ensure that the realization honors the observed values $Y(s_1), \ldots, Y(s_n)$. This can be achieved from an unconditional simulation of the random field $Y$ as follows (Lantuejoul, 2002):

1. realize a unconditional simulation $\{X(s), s \in G\}$ of the random field $Y$;
2. carried out a simple kriging of $\{X(s) - Y(s), s \in G\}$ from its values taken at the data points $\{s_i, i = 1, \ldots, n\}$, using $m(.)$ and $C^{NS}(.,.)$;
3. add the unconditional simulation and the result of kriging.

We have $Y(x) = m(x) + \sigma(x)Z(x), \forall x \in G$, where $Z$ is a Gaussian random field with zero expectation, unit variance and non-stationary correlation function $R^{NS}(.,.)$. Thus, to simulate the Gaussian random field $Y$ (step 1 of the previous algorithm), we need to known how we can simulate $Z$. Simulation of the Gaussian random field $Z$ can be carried out using a propagative version of the Gibbs sampler proposed by Lantuejoul and Desassis (2012). This algorithm allows to simulate a Gaussian vector at a large number of locations (comparatively to the existing classical algorithms such as Cholesky method or Gibbs sampler) without relying on a Markov assumption (it does not need to have a sparse precision matrix). The algorithm proposed in Lantuejoul and Desassis 2012 requires neither the inversion nor the factorization of a covariance matrix. Note that simulation methods such as spectral method or turning bands method are not adapted to the non-stationary case (Lantuejoul, 2002). The representation that underlies these methods relies on the stationarity assumption.

### 5 Application

The methodology presented in Section 4 has been applied to the elevation data of the breccia pipe called "braden" of the El Teniente mine in Chile. We have a training data (616 observations) which serves to calibrate the model and a validation data (200 observations) which serves only to assess the prediction performances. A comparison scheme of kriging under stationary and non-stationary models is carried out through a validation sample.

Raw estimates of non-stationarity parameters $m(.), \sigma^2(.)$ and $\Sigma(.)$ at anchor points are shown respectively on Figures 1b, 1c and 1d. They are based on the non-stationary exponential covariance function. Concerning the estimated anisotropy function $\hat{\Sigma}(.)$ at anchor points, it is represented by ellipses as shown in Figure 1d. Based on these estimates, non-stationarity in the data is quite visible. Especially, from Figure 1d where we can clearly see the spatially varying azimuth. Such directional effects are also quite apparent on data (Figure 1a). Note that the stationary approach has not detected a global geometric anisotropy.
Figure 1: (a) Training data; (b) Estimated mean function $\hat{\mu}(.)$ at anchor points; (c) Estimated variance function $\hat{\sigma}^2(.)$ at anchor points; (d) Estimated anisotropy function $\hat{\Sigma}(.)$ at anchor points where the ellipses were scaled to ease visualization.

Figure 2 shows the maps of smoothed parameters over the whole domain of observations: mean, variance, anisotropy ratio and azimuth. A visualization of the covariance at certain points (with all other points) via the level contours for estimated stationary and non-stationary models is presented in Figure 3. We can see how the non-stationary spatial dependence structure changes the shape from one place to another as compared to the stationary one. The stationary model is a nested isotropic model (nugget effect, exponential and spherical) while the non-stationary model corresponds to the non-stationary exponential covariance function.
Table 1 presents the summary statistics for the external validation (200 hold-out sample) results using the classical stationary approach and the non-stationary proposed one. Some well-known discrepancy measures are used (Chiles (2012)), namely the Mean Absolute Error (MAE), the Root Mean Square Error (RMSE), the Normalized Mean Square Error (NMSE), the Logarithmic Score (LogS) and the Continued Rank Probability Score (CRPS). For RMSE, LogS and CRPS, the smaller the better; for MAE, the nearer to zero the better; for NMSE the nearer to one the better. Table 1 shows that the proposed approach outperforms the stationary one with respect to all the measures. The cost of non-using the non-stationary approach in this
case is substantial: in average the prediction at validation locations is about 23% better for the non-stationary approach than for the stationary one, in terms of RMSE.

<table>
<thead>
<tr>
<th></th>
<th>Stationary</th>
<th>Non-stationary</th>
</tr>
</thead>
<tbody>
<tr>
<td>MAE</td>
<td>79.74</td>
<td>61.39</td>
</tr>
<tr>
<td>RMSE</td>
<td>154.41</td>
<td>117.99</td>
</tr>
<tr>
<td>NMSE</td>
<td>0.98</td>
<td>0.74</td>
</tr>
<tr>
<td>LogS</td>
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<td>2315</td>
</tr>
<tr>
<td>CRPS</td>
<td>123.59</td>
<td>121.11</td>
</tr>
</tbody>
</table>

Table 1: External validation on a set of 200 observations.

The kriged values and the kriging standard deviations for the estimated stationary and non-stationary models are shown in Figure 4. The overall look of the predicted values and prediction standard deviations associated with each model differ notably. In particular, the proposed method takes into account certain local characteristics (such as locally varying anisotropy) of the regionalization that the stationary approach is unable to retrieve. Figure 5 shows some conditional simulations in the Gaussian framework, based on the estimated non-stationary model.

![Figure 4](image)

Figure 4: (a,b) Predictions and prediction standard deviations for the estimated stationary model. (c,d) Predictions and prediction standard deviations for the estimated non-stationary model.
6 Conclusion

In this paper we are proposed a statistical methodology based on a non-stationary covariances class to predict the elevation of the breccia pipe elevation named ”Braden” of the El Teniente mine in Chile. The estimation method offers an integrated treatment of all aspects of non-stationarity (mean, variance, covariance) in the modeling process and relies on the mild hypothesis of quasi-stationarity. The proposed method has revealed an increased prediction accuracy when compared to the standard stationary method, and demonstrated the ability to extract the underlying non-stationarity from a single realization. It also provides an exploratory analysis tool for the non-stationarity. Beyond the spatial predictions, we also show how conditional simulations can be carried out in this non-stationary framework.

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References


