Deriving Indicator Direct and Cross Variograms from a Normal Scores Variogram Model (bigaus-full)

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The multivariate Gaussian distribution is commonly used because of its simplicity. An indicator formalism is considered when the bivariate Gaussian distribution does not fit the data. There are a number of checks for bivariate Gaussianity. Comparing the experimental indicator variograms with those from theory is the most common approach. Interest in cokriging motivated us to expand the check to indicator cross variograms. The bigaus program available in GSLIB was modified to infer the theoretical direct and cross variograms from a normal scores variogram. The calculations are performed by integration with Monte Carlo simulation. The full set of indicator direct and cross variograms at different thresholds is presented for a theoretical and a practical case. We show that a Linear Model of Coregionalization cannot be fit to the variograms from the Gaussian case; there are extraordinary low variogram values for indicator cross variograms when the two thresholds are quite different.

Introduction

Sequential Gaussian Simulation and most stochastic simulation techniques for continuous variables draw samples from a multivariate Gaussian distribution. The data are transformed to be perfectly univariate Gaussian, but it is difficult to prove the multivariate Gaussian distribution is reasonable. The normality of the univariate cumulative distribution function's (cdf) does not assure that its multiple-point distribution will be also multivariate normal (Goovaerts, 1996; Deutsch, 1998).

In practice, we check just the two-point cdf of any pair of values $Y(\mathbf{u})$, $Y(\mathbf{u} + \mathbf{h})$, $\forall \mathbf{u}, \forall \mathbf{h}$. If the spatial continuity and the two-point cdf of real data do not fit satisfactorily the bivariate Gaussian model, particularly for the extreme low and high values, a non-parametric indicator approach is considered. The experimental two-point cdf values of any set of data pairs separated by the same vector $\mathbf{h} \{(y(\mathbf{u}_{\alpha}), y(\mathbf{u}_{\alpha} + \mathbf{h}), \alpha = 1, ..., N(\mathbf{h}))\}$ match the Gaussian bivariate cdf:

$$\operatorname{Prob}\left\{Y(\mathbf{u}) \leq y_{p}, Y(\mathbf{u}+\mathbf{h}) \leq y_{p'}\right\} = G(\mathbf{h}; y_{p}, y_{p'})$$
$$= \int_{-\infty}^{y_{p}} \int_{-\infty}^{y_{p'}} \frac{1}{2\pi\sqrt{1-\rho^{2}(\mathbf{h})}} \exp\left(-\frac{y^{2}+y^{\prime 2}-2\rho_{Y}(\mathbf{h})yy^{\prime}}{2\left(1-\rho_{Y}^{2}(\mathbf{h})\right)}\right) dydy^{\prime} (1)$$
$$\forall Y(\mathbf{u}) = y, Y(\mathbf{u}+\mathbf{h}) = y^{\prime}$$

where the y_p and y_p thresholds correspond to the p and $p' \in [0,1]$ p-values, respectively, and $\rho_Y(\mathbf{h})$ is the autocorrelation function. This expression is not used for bigaussianity verification due to the difficulties in calculating this open double integral and the sensitivity of experimental proportions. Instead, the relationship between the two-point cumulative distribution and the indicator direct and cross variograms is developed to facilitate the calculations. Thus, this verification can be performed by comparing the theoretical, or Gaussian derived, indicator variogram, $\gamma_I(\mathbf{h}; p, p')$, with the experimental indicator variogram, $\hat{\gamma}_I(\mathbf{h}; p, p')$.

Until now, the direct indicator variogram case where $y_p = y_{p'}$ was deemed enough for this verification; however, Sequential Indicator full Co-Simulation requires the use of indicator cross variograms between different thresholds as a way to reduce the variability due to uncontrolled inter-classes transitions exhibited by traditional indicator based methods. A full checking of the bivariate Gaussian assumption must be performed by comparing the experimental indicator cross-variograms with the indicator cross-variograms derived from the bivariate Gaussian distribution.

The first objective of this work is to develop and test an algorithm to generate the complete matrix of indicator direct and cross variograms for multiple thresholds in order to perform the full check of bivariate normality. The second objective is to assess if a Linear Model of Coregionalization (LMC) can be fit to the resultant matrix of indicator variograms. The developed algorithm is a modification of the FORTRAN program bigauss (H. Xiao, 1975; C.V. Deutsch, 1989-1999), which is part of the GSLIB collection of Geostatistical programs and is currently used to check the bigaussian assumption by comparing the theoretical direct indicator variograms with the correspondent experimental direct indicator variograms at several thresholds.

Theoretical Framework

The multivariate Gaussian RF model is widely used by stochastic sequential simulation algorithms because it yields to an easy way to infer the parameters of the conditional cdf at any location **u**. A multivariate Gaussian RF $Y(\mathbf{u})$, with zero mean, unit variance and covariance $C_{\mathbf{u}}(\mathbf{k})$, fulfills the momenties that are stated neut (Dautach, 1008). Consumption 1000):

 $C_{Y}(h)$, fulfills the properties that are stated next (Deutsch, 1998; Goovaerts, 1996):

- All subsets of that RF, $\{Y(\mathbf{u}), \mathbf{u} \in B \subset A\}$, are multivariate normal too.
- The univariate cdf of any linear combination of the RV components of $Y(\mathbf{u})$ is normal.
- The bivariate probability distribution (or cumulative distribution function, cdf) of any pairs of RVs Y(u) and Y(u+h) is normal and fully determined by the covariance function $C_y(h)$ (Xiao, 1985; Journel and Posa, 1990):

$$F(y_{p},y_{p'},\rho_{Y}(\mathbf{h})) = \operatorname{Prob}\left\{Y(\mathbf{u}) \le y_{p}, Y(\mathbf{u}+\mathbf{h}) \le y_{p'}\right\}$$
$$= p.p' + \frac{1}{2\pi} \int_{0}^{\operatorname{arcsin}\rho_{Y}(h)} \exp\left[-\frac{y_{p}^{2} + y_{p'}^{2} - 2y_{p}y_{p'}\sin\theta}{2\cos^{2}\theta}\right] d\theta$$
(2)

Where $y_p = G^{-1}(p)$ and $y_{p'} = G^{-1}(p')$ are the standard normal quantile threshold values with probabilities p and p', respectively, and $\rho_{\gamma}(\mathbf{h})$ is the correlogram of the standard normal RF. It can be demonstrated that this expression is equivalent to the one provided in (1).

- If two RVs $Y(\mathbf{u})$ and $Y(\mathbf{u}')$ are uncorrelated, i.e., if $Cov\{Y(\mathbf{u}), Y(\mathbf{u}')\}=0$, they are also independent.
- All conditional distributions of any subset of the RF, given realizations of any other subset, are multivariate normal.

The bivariate normal probability distribution function (pdf) of the standard normal RFs $Y(\mathbf{u})$ and $Y(\mathbf{u}+\mathbf{h})$ is fully defined by its mean (zero), variance (one) and it's correlogram. This pdf can calculate by the well known expression (Anderson, 1984):

$$f(y_{p}, y_{p'}, \rho_{Y}(\mathbf{h})) = \frac{1}{2\pi} \exp\left[\frac{y_{p}^{2} + y_{p'}^{2} - 2y_{p}y_{p'}\rho_{Y}(\mathbf{h})}{2\left[1 - \rho_{Y}^{2}(\mathbf{h})\right]}\right]$$
(3)

Where the correlogram $\rho(\mathbf{h})$ is related to the corresponding variogram $\gamma(\mathbf{h})$ by the next expression:

$$\gamma(\mathbf{h}) = \frac{1}{2} E\left\{ \left[Z(\mathbf{u}) - Z(\mathbf{u} + \mathbf{h}) \right]^2 \right\} = 1 - \rho(\mathbf{h})$$
(4)

By the other side, a binary indicator transform for a continuous RF $Y(\mathbf{u})$ can be defined as:

$$I(u; p) = \begin{cases} 1 & \text{if } Y(u) \le y_p \\ 0 & \text{if } Y(u) > y_p \end{cases}, \quad p \in [0, 1]$$
(5)

The expected value of the indicator transform $I(\mathbf{u}; y_p)$ is the univariate cdf of $Y(\mathbf{u})$:

$$E\{I(\mathbf{u};p)\} = \operatorname{Prob}\{Y(\mathbf{u}) \le y_p\} = F(y_p) = p \in [0,1]$$
(6)

And its bi-variate cdf, whose analytical expression was provided in (2), is equivalent to the noncentered indicator cross-covariance, $K_I(\mathbf{h};p,p')$:

$$\operatorname{Prob}\left\{Y(\mathbf{u}) \le y_{p}, Y(\mathbf{u} + \mathbf{h}) \le y_{p'}\right\}$$

= $E\left\{I(\mathbf{u}; p) \cdot I(\mathbf{u} + \mathbf{h}; p')\right\} = K_{I}(\mathbf{h}; p, p')$ (7)

The non-centered indicator cross-covariance has the next properties:

$$K_{I}(-\mathbf{h};p,p') = K_{I}(\mathbf{h};p',p) \neq K_{I}(\mathbf{h};p,p')$$

$$K_{I}(0;p,p') = F\left(\min(y_{p},y_{p'})\right) = \min(p,p')$$
(8)

This second order moment can be calculated by integrating the bivariate Gaussian distribution over the area delimited by $Y(\mathbf{u}) \leq y_p$ and $Y(\mathbf{u} + \mathbf{h}) \leq y_{p'}$ (figure 1). This integral has no closed limits; therefore, the non centered indicator cross-covariances must be approximated by numerical methods of integration. The non centered indicator cross-covariance is related to the centered indicator cross-covariance as:

$$C_{I}(\mathbf{h};p,p') = K_{I}(\mathbf{h};p,p') - F(y_{p})F(y_{p'})$$
(9)

For cross-variogram standardization and other purposes is important to note that:

$$C_{I}(0;p,p') = K_{I}(0;p,p') - F(y_{p})F(y_{p'}) = \min(p,p') - F(y_{p})F(y_{p'})$$
(10)



Figure 1: Bivariate Gaussian distribution: The integration over the hatched areas gives the non centered indicator covariances $K_1(h;p,p')$ and $K_1(h;p',p)$, respectively.

 $E\{I(u; p) \cdot I(u; p')\} + E\{I(u+h; p) \cdot I(u+h; p')\} - E\{I(u; p) \cdot I(u+h; p')\} - E\{I(u+h; p) \cdot I(u; p')\}$



Figure 2: The Gaussian indicator variogram in terms of volumes under the bivariate Gaussian distribution

From Equation (7), the Gaussian indicator cross-variogram can be defined in terms of the noncentered covariance as:

$$2\gamma_{I}(h; p, p') = E\left\{ \left[I(u; p) - I(u + h; p) \right] \left[I(u, p') - I(u + h; p') \right] \right\}$$

= 2K_I(0; p, p') - K_I(h; p, p') - K_I(h; p', p) (11)
= 2 min(p, p') - K_I(h; p, p') - K_I(h; p', p)

This expression can be understood in terms of a difference of volumes under the bivariate normal distribution surface, limited by the thresholds y_p and $y_{p'}$ (see Figure 2). These volumes are equivalent to the univariate and bivariate cumulative probabilities for these thresholds. The Gaussian indicator cross-variogram can also be calculated analytically from (2), (8) and (11) as:

$$2\gamma_{I}(h; p, p') = 2\min(p, p') - 2p \cdot p' - \frac{1}{2\pi} \int_{0}^{\arcsin C_{Y}(h)} \exp\left[-\frac{y_{p}^{2} + y_{p'}^{2} - 2y_{p}y_{p'}\sin\theta}{2\cos^{2}\theta}\right] d\theta$$
(12)
$$-\frac{1}{2\pi} \int_{0}^{\arcsin C_{Y}(-h)} \exp\left[-\frac{y_{p}^{2} + y_{p'}^{2} - 2y_{p}y_{p'}\sin\theta}{2\cos^{2}\theta}\right] d\theta$$

Consequently, in order to check the multigaussian assumption, the results of the expressions (11) or (12) can be compared graphically, for each pair of threshold values, with the experimental indicator cross-variogram of normal score data, which is computed as:

$$2\hat{\gamma}_{I}(h;p,p') = \frac{1}{N(h)} \sum_{\alpha=1}^{N(h)} \left[I(u_{\alpha};p) - I(u_{\alpha}+h;p) \right] \left[I(u_{\alpha};p') - I(u_{\alpha}+h;p') \right]$$
(13)

Implementation

Currently, bigauss program derives the Gaussian indicator direct variograms, i.e. when p=p', using a non-recursive adaptive integration algorithm, which is a modification of the Simpson's rule, to perform a numerical integration of the non centered indicator covariance, which is expressed as:

$$K_{I}(h;p) = \operatorname{Prob}\left\{Y(\mathbf{u}) \le y_{p}, Y(\mathbf{u}+\mathbf{h}) \le y_{p}\right\}$$
$$= p^{2} + \frac{1}{2\pi} \int_{0}^{\arcsin\rho_{Y}(h)} \exp\left[\frac{-y_{p}^{2}}{1+\sin\theta}\right] d\theta$$
(14)

The results of this numerical integration are used to derive the correspondent theoretical Gaussian indicator direct variogram. In the implementation of bigauss2 program (P.C. Kyriakidis, C.V. Deutsch, and M.L. Grant, 1999) the Simpson's rule algorithm was changed for a power series expansion approach. The implemented algorithm computes the coefficients for the power series approximation of the centered indicator cross-covariance, $C_I(\mathbf{h};p)$, derived from the bivariate Gaussian distribution which is defined by the continuous variable covariance, $C_y(\mathbf{h})$. Afterwards, the calculation of the theoretical indicator direct variogram is straightforward.

A possibility for the implementation of bigauss-full would be to modify the algorithms used in the actual programs bigauss or bigauss2 in order to integrate numerically the theoretical indicator cross-covariances defined by the expression (12). Nevertheless, instead of trying these option, another approach has been followed because its straightforward implementation, that is, we calculate the non-centered cross-covariances, $K_{I}(h; p, p')$ and $K_{I}(h; p', p)$ numerically using Monte Carlo Simulation for the integration. We randomly generate a large number of $(Y(\mathbf{u}), Y(\mathbf{u} + \mathbf{h}))$ points in the bivariate Gaussian space defined by expression (3), and then to compute the density of these several thousand random points in the areas defined in Figure 1 as the values of the non-centered crosscovariances. This iterative procedure implemented in bigauss-full follows the steps described next:

- a) Select two thresholds y_p and $y_{p'}$ in normal space.
- b) Draw a random number $p_1 \in [0,1]$, and calculate $Y(u) = G^{-1}(p_1)$
- c) Draw a second random number $p_1 \in [0,1]$, and calculate the associated value $Y(u+h) = G_{(\mu,\sigma)}^{-1}(p_2)$ from the conditional bivariate distribution with conditional mean (μ) and variance (σ):

$$\mu_{Y(u+h)/Y(u)} = \rho(h)Y(u) \tag{15}$$

$$\sigma_{Y(u+h)/Y(u)}^{2} = 1 - \rho^{2}(h)$$
(16)

- d) Check: $Y(u) \le y_p$ and $Y(u+h) \le y_{p'}$, if this condition is satisfied add one to a first counter N₁.
- e) Also check: $Y(u) \le y_{p'}$ and $Y(u+h) \le y_p$, if this is satisfied, add one to the second counter N₂.

The inner loop from steps b to e is repeated several thousand times in order to obtain enough points for smooth Gaussian variograms, the outer loop, from steps a to e, is repeated for all the thresholds combination included when $y_p = y_{p'}$. For each pair of thresholds, the two non centered indicator cross-covariances are calculated at the end of the inner loop iterations as the division of the counters N₁ and N₂ by the number of iterations, respectively. Subsequently, the corresponding theoretical Gaussian indicator variogram is calculated using the expression (11).

Program Description

bigauss-full uses the same parameter file as the old bigauss program (fig 3), nevertheless, the new program generates not only the direct theoretical indicator cross-variograms, but the full matrix of indicator direct and cross-variograms. The output file contains the standardized and non-standardized values for the indicator direct and cross-variograms. Two versions of bigauss-full were built, the version 1 gives and output file with the old variogram format, the output file of version 2 has the same format as gamv2004 program and

the variograms generated can be used by the new varfit_ind_cont program for fitting a Linear Model of Coregionalization.

Program Testing

Two tests were performed for the bigauss-full results. The first test was undertaken using two hypothetical variogram models, in order to understand the behavior of the Gaussian indicator variogram using very simple variogram models. The second test was done using real data to check the concordance of the real data distribution with the bivariate Gaussian assumption.

START OF PARAMETERS: bigaus-full-cu.out 3		-file for output of variograms -number of thresholds
0.25 0.50 0.75 2 70		
120.0 0.0 5		-azm(1), dip(1), lag(1)
30.0 0.0 5		-azm(2), dip(2), lag(2)
1 0.25		-nst, nugget effect
1 0.75 120.0 0.0 280.0 140.	0.0 .0 10.0	-it,cc,ang1,ang2,ang3 -a_hmax, a_hmin, a_vert

Figure 3: Parameter file for Bigauss-Full program.

For the first test, two different variogram models were used, the first one was a spherical model with range and sill equal to one, and the second one was also spherical with sill and range equal to one, but with 0.3 nugget effect. For the sake of verification of results, in Figures 4 and 5 (at the end of the paper) the resultant standardized Gaussian indicator variograms were plotted together with the Gaussian direct variograms (solid curves) generated by the old bigaus program; the results coincide. The hypothetical continuous variogram model was also plotted, in dashed lines, together with the Gaussian derived indicator variograms for comparison purposes. The areas over which bigaussian distribution function was integrated to obtain each indicator variograms represent were also plotted as dashed areas in the bigaussian plot. Note that for the cross-variograms with extreme threshold values the resultant curves are not so smooth, this is because the applied Monte Carlo simulation produces a much lower number of random values in the extremes of Gaussian distribution. This can be alleviated with a greater number of iterations, but at the expense of increasing considerably the CPU time.

For the second test, real data from a single bench of a Chilean copper deposit was used to calculate the experimental variograms and fit a continuous variogram model. This model was introduced to bigauss-full in order to calculate the theoretical indicator variograms for the thresholds correspondent to the p-values 0.25, 0.50 and 0.75 in the major and perpendicular anisotropy directions. In Figures 6 and 7 the experimental non-standardized and standardized indicator variograms are plotted together with the indicator variograms generated from the bigaussian model and the gaussian direct indicator variograms from the old bigauss program.

Discussion

As it can be observed in Figures 4 and 5, the Gaussian indicator variograms changes their shape as the difference between the thresholds increases, from close to the exponential model for similar thresholds, to a shape akin to the Gaussian model when the thresholds are different. The variogram sills become smaller as the difference between thresholds increases, this variation can be understood and calculated from the Equation (10).

The most significant feature is the extreme continuity of the cross indicator variogram of widely separated thresholds, it is reflected in a long tail of zero and close to zero variogram values for short distances, and can be observed not only in the Gaussian derived indicator cross variograms, but also in the experimental ones (see Figures 6 and 7), becoming more important when the nugget effect of the continuous variogram approaches zero.

This extraordinary continuity can be explained in regard to the bigaussian distribution graphs in the Figures 4 and 5 where the volumes over the areas delimited by the thresholds become smaller as thresholds diverge. If the correlation which defines the bivariate Gaussian distribution increases at short distances \mathbf{h} , the bigaussian surface gets very narrow around the 45 degrees line and the volumes that define the indicator cross variograms approaches zero.

This feature can be also understood by realizing that the indicator cross-variogram registers the transition from the class defined by the first threshold to the class defined by the second one for different modulus and directions of the vector h, therefore, when the RV is very continuous and the two thresholds are very different among them, so few class transitions are found for short ranges, thus the indicator variogram becomes zero or very close to zero at such close distances. Inversely, when both thresholds are similar more transitions appear at shorter distances, producing an increased nugget effect. Experimental Indicator direct and cross variograms generated with real data can also present these features (Figures 6 and 7), although they can be masked by intrinsic patterns of spatial distribution reflected in the experimental variograms.

Due to the characteristics explained above, the resultant matrix of indicator direct and cross variograms can not be fitted satisfactorily using a Linear Model of Corregionalization (LMC). An attempt to do it is shown in Figure 8, where it can be observed that even though the direct variograms are fitted acceptably, the model approximation to the indicator cross-variograms is very unsatisfactory.

Any further attempt to fit the complete set of variograms in a standard way would not accomplish the necessary conditions of a permissible LMC, which are (P. Goovaerts, 1997):

- 1. The functions $\gamma_{ii}(h)$ are permissible variogram models, and
- 2. All the corregionalization matrices are all positive semi-definite.

The first condition can not be accomplished because the indicators cross-variogram for extreme divergent thresholds cannot be fitted adequately with a permissible variogram model (see Figure 9). The indicator direct variograms and indicator cross variograms for less divergent thresholds can be fitted individually and reasonably well with models of the family of the Stable Variograms, which include the Gaussian and Exponential variograms (Chilès & Delfiner 1999):

$$\gamma(h) = 1 - \exp\left(-\left(\frac{h}{a}\right)^{\alpha}\right) \qquad a > 0, \ 0 < \alpha \le 2$$
(16)

But cross variograms for widely separated thresholds require values of the α exponent bigger than 2, which yield to not allowable models.

Nevertheless, even if the first condition could be satisfied for individual indicator direct or cross variograms, the second condition could not. This is because one of the rules to assure positive semi-definiteness of the correlation matrix under the LMC states that every basic structure appearing on a cross variogram must be also present in the direct variograms maintaining the

same range and only changing its contribution. The changing shape of the variograms in this matrix does not allow fulfilling this rule.

Since these variograms are the result of the licit bivariate Gaussian distribution, the positive definitiveness could be demonstrated; however this exceeds the scope of the work and could lead to the development of a non linear model of corregionalization.

For the real data indicator variograms of Figures 6 and 7 it can be observed that, for this particular data set, there is an acceptable match in terms of sill and range between the experimental and theoretical indicator direct and cross variograms for most of p-quantiles combinations, this suggest the adequacy of the multigaussian assumption if this data set is used for Gaussian based grade modeling algorithms. Nevertheless there are some exceptions, the most obvious ones are given by the direct experimental variograms correspondent to the p=p'=0.25 and p=p'=0.75 quantiles, which present shorter ranges and different sills than the theoretical variograms. These divergences are expected due to different patterns of correlation for low or high values, and highlight the capability of indicator based methods to deal with relatively complex spatial features.

Conclusions

- The bigauss-full program generates the Gaussian derived indicator direct and cross-variograms; however, the resultant matrix of indicator direct and cross variograms can not be fitted satisfactorily by a classic Linear Model of Coregionalization.
- An important feature that makes this fitting impossible is the extraordinary continuity of indicator cross variograms of widely separated thresholds.
- Further research is needed to develop an adequate model of coregionalization in order to use consistently the indicator cross variograms in indicator cokriging and cosimulation.
- The comparison of experimental indicator direct and cross variograms with the corresponding Gaussian variograms is useful to assess the adequacy of the multigaussian model. When dissimilarities between experimental and Gaussian derived variograms, particularly for very high and very low values, are evident then an indicator approach is more suitable than the Gaussian approach to handle with the complexity of spatial variability at different thresholds.

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Figure 4: Gaussian derived indicator variograms and a spherical model of sill and range equal 1.





Figure 6: non-standardized Gaussian and experimental indicator cross and direct variograms.



Figure 7: Standardized Gaussian and experimental indicator cross and direct variograms.



Figure 8: Fitting of a Linear Model of corregionalization to the matrix of Gaussian derived indicator direct and cross variograms.



Gaussian Indicator Variogram Fitting

Figure 9: Individual fitting of the Gaussian derived indicator cross variogram of two extreme thresholds. Note that the Gaussian model gives a very coarse approximation and it is not enough to describe the high continuity at short distances.