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Statistical tool for soil biology X. Geostatistical analysis

Jean-Pierre Rossi, Patrick Lavelle and Jérôme Ebagnerin Tondoh

Laboratoire d'Écologie des Sols Tropicaux. ORSTOM/Université Paris 6, 32, av. Varagnat, 93143 Bondy Cedex, France.

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Abstract

Soil living organisms currently exhibit complex spatial patterns at various scales. Conventional methods for studying spatial dispersion are based on various aggregation indices or probability distribution analysis. Since these methods do not take into account the actual location of the sampling sites, they provide no information on the spatial distribution at scales larger than the sampling unit size. The geostatistical analysis is a way to analyse the spatial pattern of a variable at scales ranging from the minimum to the largest inter-sample distance. The variogram indicates whether the variable is spatially dependent or not. If a structure is present, the kriging local interpolation procedure provides estimates of the variable and their estimation error. Contour mapping of these values gives accurate maps of both the variable and the reliability of the estimated values. Kriging is a local estimation method that yields fine description of short and large-scale structures whereas traditional interpolation procedure by trend surface analysis only describes large-scale patterns. At a further stage, the relationship between two spatially dependent variables can be examined by cross-variogram analysis. The latter procedure allows the study of the complex relationships that occur either between biological variables or biological and environmental variables.

Keywords: Geostatistics, variogram, kriging, earthworm, spatial distribution, trend surface analysis.

L'outil statistique en biologie du sol. X. Analyses géostatistiques.

Résumé

Les organismes du sol présentent généralement des patrons de distribution spatiale à divers échelles. Les méthodes classiques d'étude de la distribution spatiale sont basées sur divers indices d'agrégation ainsi que sur l'analyse des distributions de fréquence. Ces méthodes ne prennent pas en considération la position des points d'échantillonnage et par conséquent n'apportent pas d'information sur la distribution spatiale des organismes aux échelles supérieures à l'unité d'échantillonnage. L'outil géostatistique permet la description de la distribution spatiale d'une variable à l'intérieur de l'aire d'échantillonnage. Le variogramme indique si la variable présente une structure spatiale et dans ce cas, l'utilisation du krigeage, méthode d'interpolation locale, fournit à la fois une estimation de la variable ainsi que son erreur d'estimation. Le krigeage est une méthode d'interpolation locale autorisant une description précise des structures fines impossible à obtenir par la méthode traditionnelle d'analyse de tendance. Les relations entre deux variables structurées dans l'espace peuvent être étudiées par l'analyse du covariogramme. Cette méthode permet l'étude des relations complexes qui interviennent entre différentes variables biologiques ou entre variables biologiques et variables environnementales.

Mots-clés : Géostatistiques, variogramme, krigeage, vers de terre, distribution spatiale, analyse de tendance.

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INTRODUCTION

Soils are highly heterogeneous environments as a result of the large number of factors that determine their structure and regulate their function. Following the hierarchy theory (Allen & Starr, 1982) soils can be seen as primarily structured by large-scale physical processes that create large-scale structures within which smaller scale contagious biotic processes introduce a new level of heterogeneity.

Soil living organisms currently exhibit complex spatial patterns at various scales. Plant parasitic nematode populations are spatially dependent at scales of <1 m (Rossi *et al.*, 1995a) to 80 m (Robertson & Freckman, 1995) or 180 m (Wallace & Hawkins, 1994). Earthworms too have characteristic patterns of spatial distribution at scales ranging from 1 m (Rossi J. P., unpublished) to 50 m (Poier & Richter, 1992). These patterns are either due to internal processes in populations or to the influence of environmental patchiness or a combination of both effects.

Conventional methods used to assess the spatial pattern of soil organisms basically separate three types of distributions *i. e.*, random, regular and aggregated (clumped). These methods are based on quadrat counts and can be divided in two major categories.

The first approach consists in fitting a discrete probability distribution to sample count frequency data and indicates whether the distribution is random or not. In the case of clumped distributions, sample frequency distribution often fits a negative binomial model while random patterns lead to a Poisson distribution. Regular patterns that follow the positive binomial model are extremely rare in soil organisms. The distribution parameters are estimated from frequency table by the maximum likelihood procedure and a chi-square goodness-of-fit is used to determine whether the observed data significantly differ from the fitted distribution.

A second approach is based on the computation of various indices of dispersion measuring the degree of non-randomness in spatial patterns. A wide range of indices is available from the literature (Taylor, 1961; Cancela da Fonseca, 1966; Lloyd, 1967; Chessel, 1978; Cancela da Fonseca & Stamou, 1982). Among them, the variance to mean ratio and the Taylor's power law are frequently met in literature (Cancela da Fonseca, 1966; Elliot, 1971; Boag & Topham, 1984; Ferris *et al.*, 1990; McSorley & Dickson, 1991). Departure from randomness of these indices can be tested using appropriate statistics.

The negative binomial parameter or its inverse are often used as a dispersion index provided the negative binomial fits the data (Cancela da Fonseca, 1965; 1966; Elliot, 1971). This approach has been largely used although Taylor *et al.* (1979) showed severe ecological restrictions of that index.

However, the interpretation of the index values often depends on the relative size of aggregates and sampling units: aggregation is adequately measured if samples and aggregates are of comparable sizes. When samples are significantly larger than aggregates, the index measures the aggregation of smaller aggregates. If samples are much smaller than aggregates, aggregation cannot be demonstrated (Chessel, 1978).

Further, examination either of the indices or frequency distributions carries limited information since these methods do not take into account the actual location of sampling points with respect to each other. These approaches are de facto limited to the analysis of the organisms distribution within the sampling units. Assessing patterns at larger scales requires taking into account the spatial location of sample points inside the investigated surface. Basically, a variable is said to be regionalized or autocorrelated if a measure at one point carries information relative to neighbouring points. If autocorrelation is present among data, conventional statistics are no longer valid. As an example, the Pearson correlation coefficient cannot be used (Legendre, 1993) and other methods must be applied.

Furthermore, available data sets show that biological variables are rarely spatially independent at a field scale of <100 m (Robertson, 1994). Thus soil ecologists need tools to quantify the spatial dependence over various spatial scales. Geostatistics specifically address these issues. They constitute a group of mathematical treatments that were developed with the object to describe quantitatively the spatially structured (*i. e.* autocorrelated) variables. These methods Matheron (1965, 1971) have been increasingly used in soil science since the early 80's.

With the development and diffusion of microcomputer software (Robertson, 1987; Yost *et al.*, 1989), geostatistics have been largely used in studies of spatial patterns of soil physico-chemical variables. Their introduction in soil ecology is recent (Robertson, 1987, 1994; Webster & Boag, 1992; Wallace & Hawkins, 1994; Delaville *et al.*, 1995a, b; Robertson & Freckman, 1995; Rossi *et al.*, 1995a, b).

DETECTION AND DESCRIPTION OF SPATIAL STRUCTURES BY GEOSTATISTICS

Geostatistical analysis is a two-step procedure. First, the spatial structure of the variable is examined with the semi-variance analysis. Once a spatial structure has been identified and accurately described by a suitable model, the kriging procedure provides optimal interpolation of the variable at unsampled sites.

Semi-variance analysis and the variogram

The variogram allows the study of the autocorrelation phenomenon as a function of the distance. It is an univariate method limited to quantitative variables. Before estimating the variogram, one must

ensure that data follow the "intrinsic hypothesis" that assumes that the differences between all pairs of points located a given distance apart have constant mean and variance throughout the sampled surface. This relaxed form of stationarity assumption makes possible the use of semi-variance analysis for ecological studies.

However, if a large-scale structure is present it will be picked up by the variogram and finer spatial patterns may be masked. Large-scale spatial trends should then be removed using regression (trend surface analysis) prior to variogram computation. Analysing the residuals may allow to investigate the finer structures.

Variations of a variable that changes in a continuous manner from point to point can be described by a mathematical function: the semi-variance (Equation 1).

The semi-variance (γ) is estimated at each distance interval h and the resulting graph of γ against the lag h is called the semi-variogram or variogram for convenience. At lag h, the semi-variance is half the expected squared difference between recorded values a distance h apart (Equation 1).

$$\gamma(h) = 1/2\,M(h) \sum_{i=1}^{M(h)} \{[Z(x_i) - Z(x_i + h)]^2\} \quad (1)$$

Where $M(h)$ is the number of comparisons at lag h and $Z(x_i)$ and $Z(x_{i+h})$ the values of that variable at any two places separated by the lag h.

The lag h is a vector defined with both distance and direction. Practically, the effect of direction (anisotropy) is examined by estimating the variogram along several directions (Burgess & Webster, 1980a). The resulting graphs are compared and if no significant differences are found, variations are considered as isotropic. If not, the kriging algorithms have to be modified (Burgess & Webster, 1980a; Webster, 1985).

A few general features of the variogram must be mentioned. Generally curves are bounded, $\gamma(h)$ increases with h until a certain value of h called the range (a) after which the semi-variance is maximum and remains constant. This semi-variance value called the sill theoretically equals the variance of the data set. Couples of data separated by a distance less than the range are statistically dependent (*i. e.* measure at a given point carries information on the expected value at another point a distance lower than the range apart). Independence between points is thus achieved if distance separating these points is higher than the range (Burgess & Webster, 1980a, b; Yost *et al.*, 1982a).

Another feature of the variogram is the "nugget effect". If theoretically, $\gamma(h) = 0$ when $h = 0$, in practice it is rarely observed. Generally the intercept is a positive value called the nugget variance (C_0). This reveals the presence of a residual variation at the shortest sampling interval.

The nugget variance is the sum of two sources of variation: the measurement errors (also referred to as the *human nugget*), and variations within the sampling interval. The difference between the sill and C_0 is called the structural or spatial variance (C). It is the part of total variance that can be attributed to the spatial autocorrelation (see *fig.* 1). Many sample variograms exhibit 100% nugget variance and are flat (Wallace & Hawkins, 1994; Robertson & Freckman, 1995). This means that no spatial structure is detected. However, changing the scale of observation may reveal unseen patterns (Burrough, 1983).

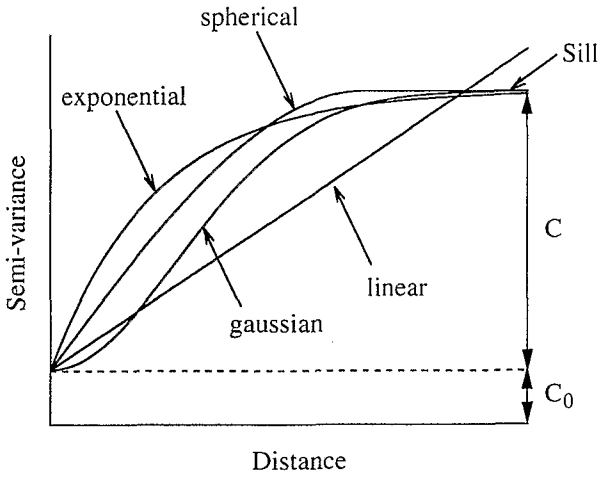

Figure 1. – Four common theoretical models for variograms. C_0 = nugget variance and C = structural variance.

Semi-variogram modelling

The semi-variance analysis is an attempt to fit a mathematical function to the semi-variance values estimated at distance interval of increasing values. The model parameters are used in kriging interpolation method.

Not all functions that seem to fit the observed values will serve. The variogram function must be "conditional negative semi-definite" (CNSD) (Armstrong & Jabin, 1981). Since testing the positive definiteness is tedious, geostatisticians use several common "approved" models and eventually combine them to provide better fit (Webster, 1985). These models are called "authorized" functions. *Figure* 1 shows the most common models. There are two classes of models: bounded models that exhibit a plateau (the sill) and unbounded models where variance appears to increase without limit.

Unbounded models

The simplest unbounded model is the linear model (*fig.* 1). Semi-variance increases with distance following the linear relationship:

$$\gamma(h) = C_0 + wh$$

Where h is the distance, C_0 the nugget variance and w the slope. A straight line is fitted to the observed values, the intercept being the nugget variance (C_0) .

Bounded models

The most common bounded model is the spherical model (*fig.* 1). The function is:

$$\gamma(h) = C_0 + C\left\{\frac{3h}{2a} - \frac{1}{2}\left(\frac{h}{a}\right)^3\right\} \quad \text{for} \quad h < a$$

$$\gamma(h) = C_0 + C \quad \text{for} \quad h \geq a$$

Where h is distance, C_0 the nugget variance, C the spatial variance (sill minus nugget variance) and a is the range. When distance equals the range, the semi-variance reaches the sill.

The exponential model accurately described physico-chemical data (e.g. Yost *et al.*, 1982a; Voltz, 1986; Oliver & Webster, 1987) and biological variables (nematode density, Rossi *et al.*, 1995a). Formula is:

$$\gamma(h) = C_0 + C\{1 - \exp(-h/r)\}$$

r is a distance parameter that defines the spatial scale of the variation. The sill is approached asymptotically and there is no strict range. Nonetheless, a common rule of thumb is to take the effective range as $a' = 3r$ which is the inter-sample distance at which the semi-variance reaches approximately $C_0 + 0.95\ C$ (Webster, 1985) (see *fig.* 1).

In some occasions, the linear model may be bounded. As distance between sample locations increases, the semi-variance remains constant and equal to the sum of nugget *plus* spatial variance. This model is an authorized function only in one dimension (Webster & Oliver, 1990).

Fitting procedure

Choosing and fitting a theoretical model to the sample variogram is an important step of geostatistical analysis (McBratney & Webster, 1986). Least squares methods are widely used as fitting procedures. The weight applied to each of the semi-variance estimates is proportional to the number of couples of data involved in that estimate (Cressie, 1985; McBratney & Webster, 1986). Cressie (1985) proposed a fitting procedure that takes into account the different numbers of data pairs involved in each semi-variance estimate and that gives more weight to estimates at smaller distances.

Cross-variogram

Two variables are defined as cross-correlated if the value of one at a given location depends (in a statistical sense) on the values of the other at nearby locations (Myers, 1982; McBratney & Webster, 1983; Warrick *et al.*, 1986). Such variables are also named coregionalized with reference to the regionalized theory of Matheron. Cross-variogram analysis is a spatial analysis technique in which two variables are used with the aim to examine the spatial co-structure occurring between them.

Thus, coregionalization and cross-variogram are adequate tools to study inter-relationships between physico-chemical variables, organisms and physico-chemical variables or indeed, different species density (Rossi R. E. *et al.*, 1992). Let V and W be two spatially structured variables. Their spatial interdependence can be expressed in the cross semi-variance estimated as:

$$\hat{\gamma}_{vw}(h) = \frac{1}{2N(h)} \sum_{i=1}^{N(h)} [V(x_i) - V(x_i+h)]\,[W(x_i) - W(x_i+h)]$$

Where $N(h)$ is the number of all possible data pairs separated by a distance h. The cross-variogram is the plot of cross semi-variance against the distance h. It shows the same features as those of auto-variogram except that cross semi-variance is susceptible of being negative if there is a negative correlation between variables (McBratney & Webster, 1983).

Fitting theoretical model to sample cross-variogram is done using the current procedure (Cressie, 1985) used with auto-variogram.

Example 1: Field distribution of an earthworm population.

To illustrate the use of the variogram we shall take a data set collected in an African grass savanna in July 1994 (Rossi J. P., unpublished). 100 sampling points were regularly distributed on a square grid with 5 m side. At each sample location a $25 \times 25 \times 10$ cm soil monolith was taken and earthworms were handsorted. In this example, we analyse the spatial pattern of the earthworm *Chuniodrilus zielae* (Eudrilidae) population. Count frequency was highly skewed to left (*fig.* 2) and data were Ln transformed before any computation. The transformation applied was $\mathrm{Ln}(1 + x)$ since the observed earthworm density was zero at some sampling points.

The variogram was computed with the programme VAR5 which is part of the geostatistical package developed by the University of Hawaii (Yost *et al.*, 1989). A spherical model was fitted to the estimated variogram. Model parameters are: nugget variance $(C_0) = 0.7$, structural variance $(C) = 1.53$ and range $a = 23.9$ m. The relative structural variance

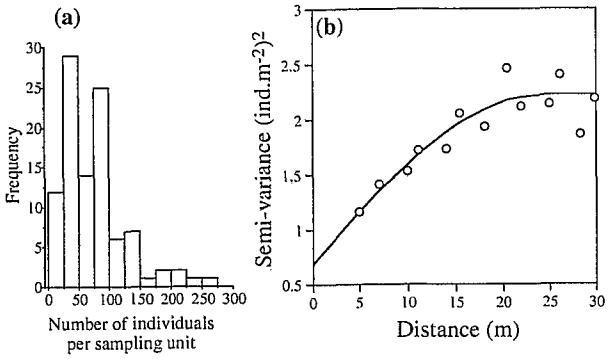

Figure 2. – (a) Frequency distribution of the density of *Chuniodrilus zielae* (Eudrilidae); (b) Variogram of the density of *Chuniodrilus zielae* (Eudrilidae) after $\mathrm{Ln}(1+x)$ transformation.

$(C/(C+C_0))$ is high (67.7%) and represents the part of the variance that can be attributed to spatial autocorrelation. The relative nugget variance $(C_0/(C+C_0))$ is the remaining variance (32.3%). This unexplained spatial variability is either random or expressed at scales below the minimum inter-sample distance (5 m in the example). The variogram reveals the presence of a spatial autocorrelation at a scale of 5m to ca. 24 m (the range).

Example 2: Absence of a spatial structure.

When no spatial pattern is perceived the variogram exhibits a 100% nugget effect. The variogram is "flat" as the semi-variance fluctuates around sample variance; there is no structural variance. *Figure* 3 represents the sample variogram for the density of the tropical earthworm *Millsonia anomala* (Megascolecidæ) in a grass savanna of Côte d'Ivoire (the sampling site and scheme are the same as in example 1). At the scale of the investigation, the observation of a 100% nugget variance variogram means that the spatial distribution of *M. anomala* is uniform throughout the sampled domain. However, changing the scale of the sampling scheme may reveal unseen patterns *i. e.* short-scale patterns.

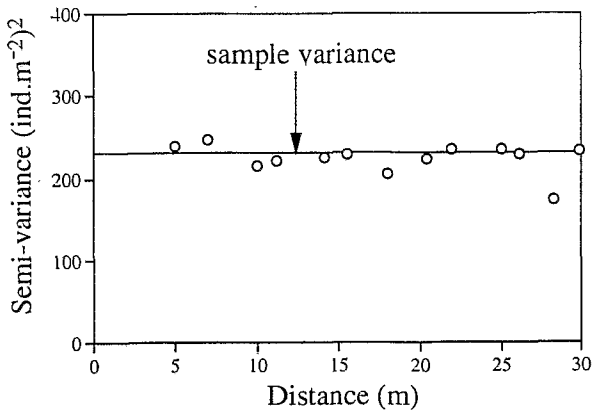

Figure 3. – Variogram of the earthworm *Millsonia anomala* density showing the absence of structure (100% nugget variance).

Example 3: Cross-correlation.

The use of the cross-variogram is illustrated with the *M. anomala* data set collected in a grass savanna (see example 2). In example 2 no consistent spatial pattern was observed for a population of *M. anomala.* However, both adult and juvenile stages produced a spherical variogram showing the presence of spatial patterns.

If both adults and juveniles are spatially dependent variables while the sum appears as spatially independent, the patterns displayed by adults and juveniles may be opposed leading in turn to a global "homogeneous" distribution of the species throughout the study field.

A cross-variogram was calculated between adult and juvenile density (*fig.* 4). The cross semi-variance values and the slope of the cross-variogram were negative, hence indicating a negative coregionalization.

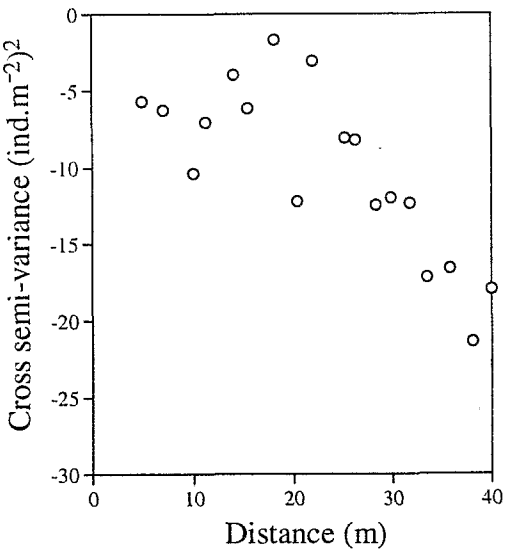

Figure 4. – Cross-variogram for the adult versus the juvenile stage of the earthworm *Millsonia anomala.*

The cross-variogram constitutes an interesting alternative to conventional Bravais and Pearson correlation coefficient since the later is not applicable to spatially dependent variables (Legendre & Troussellier, 1988; Legendre, 1993). In soil ecology, this tool has been used to investigate the relationships between different plant parasitic nematode species in a sugarcane by Rossi *et al.* (1995a).

Interpolation and mapping

Mapping is the starting point of many studies of spatially structured phenomena. Maps generally derive from samples obtained from the investigated surface

and intermediate values are estimated by interpolation. Contouring algorithms are used to draw maps from the fine grid of interpolated points.

Trend surface and Kriging

Trend surface analysis consists in fitting a polynomial equation to the x and y sample locations by regression. The larger the order of the polynomial the better the fit. However, these parameters become more and more difficult to interpret ecologically. The polynomial equation provides estimates of the variable at unsampled sites that are used to draw contour maps. Furthermore, residuals from measured and estimated values can be used to draw maps representing the variation not expressed by the interpolated map.

Kriging is a local interpolation method that produces more detailed map than ordinary interpolation. It uses data points located in the vicinity of the point where estimation is to be done and the autocorrelation structure of the variable as described by the variogram. Kriging provides an estimated value and the estimation standard deviation at non-sampled sites. Punctual kriging provides estimates for a volume exactly equalling the one of samples while block kriging gives estimates of the average value for a given volume, generally several times larger than the sampling units.

Let Z be a regionalized variable and $Z(x)$ its realization at point x. Consider n sampling points available in surrounding neighbourhood. It is possible to estimate the value of Z at site x_0 by the linear sum:

$$Z^*(x_0) = \sum_{i=1}^{n} \lambda_i Z(x_i)$$

With λ_i the weights applied to each of the i recorded values $Z(x_i)$ within the neighbourhood.

The first requirement of kriging is that estimates are unbiased.

This means that $Z^*(x_0) = E[Z(x_0)]$.

Consequently, weights must sum to 1:

$$\sum_{i=1}^{n} \lambda_i = 1$$

In addition, the variance of the estimation error (the kriging variance) is minimized with respect to λ_i that sum to 1.

The weights λ_i are derived from a set of equations determined by variogram model parameters and the location of sampling points relative to the point where estimation is to be done (Webster & Burgess, 1980b; Yost *et al.*, 1982b).

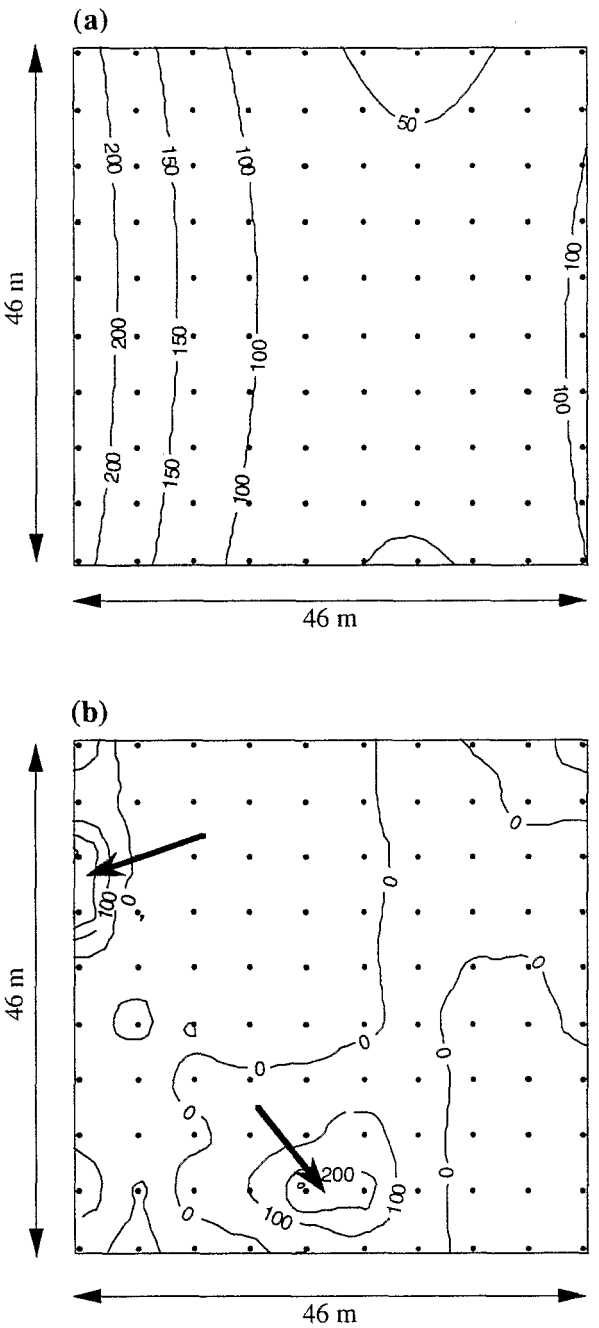

Figure 5. – (a) Contour map of the density of *Chuniodrilus zielae* (Eudrilidae) obtained by trend surface analysis; units are individuals/m^2 (b) Contour map of the residuals; units are individuals/m^2. Arrows indicate local high values of the residuals that show the ineffectiveness of the polynomial equation to describe the earthworm population local structures. •: sampling points.

Example 4: Mapping earthworm density by trend surface analysis and kriging

Trend surface analysis and block kriging were applied to the earthworm data of example 1. A 3d order polynomial was fitted to the data ($r = 0.68$; $p < 0.01$). The resulting polynomial equation was used

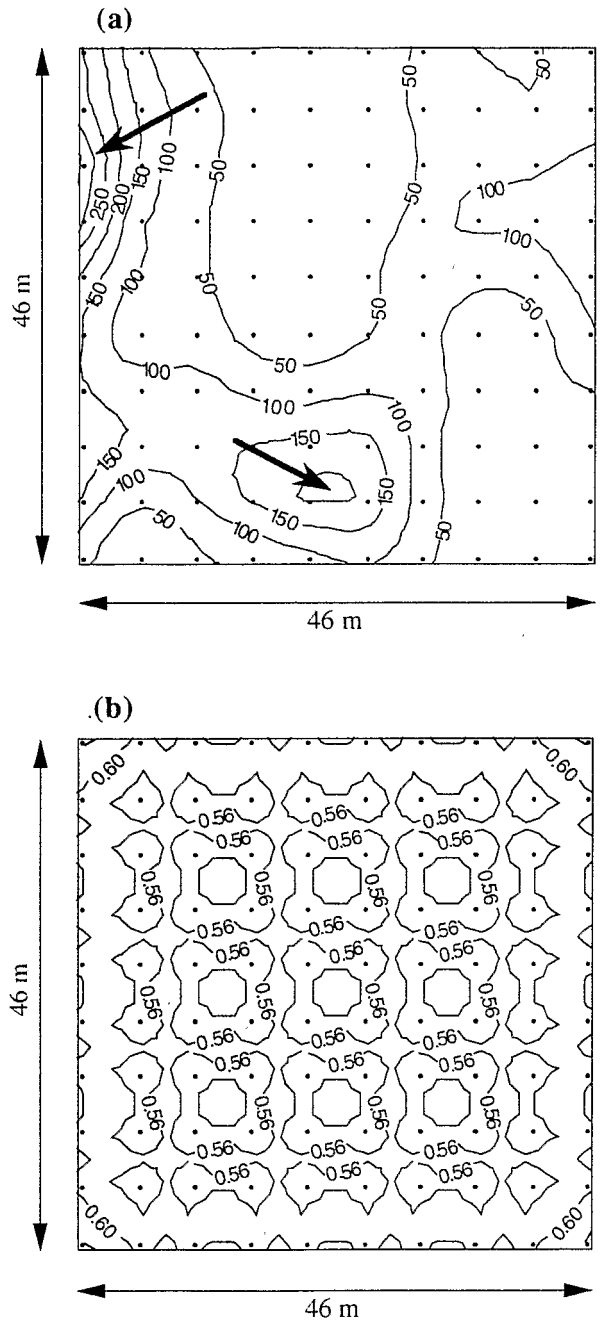

Figure 6. – (a) Contour map of the density of *Chuniodrilus zielae* (Eudrilidae) obtained by kriging; units are individuals/m^2 (b) Contour map of the kriging standard deviations; units are individuals/m^2. Arrows indicate short-scale spatial structures that were not accounted for by the trend surface analysis. •: sampling points.

to estimate earthworm density at unsampled points located on a square grid (2 m side) superimposed on the sampling scheme. At the same location, density was estimated by block kriging with 2 × 2 m blocks.

Figure 5a illustrates the contour map obtained with estimates by polynomial estimation. *Figure* 5b is the map of the residuals of the regression showing the earthworm density that is not expressed by the trend surface map. *Figure* 6a represents the contour map of the earthworm density estimated by block kriging and *figure* 6b the kriging error. As data set was Log-transformed prior to variogram computing and kriging estimation, the estimates were back-transformed before contour mapping. Kriging standard deviations were left expressed in the Log scale.

The contour map obtained with estimates by polynomial estimation (*fig.* 5a) is crude compared to map from kriging estimates (*fig.* 6a). Only large-scale patterns are represented with trend surface analysis as short-scale structures (arrows in *figs.* 6a and 5b) can only be described by a local estimation technique. Since the trend surface analysis is based on a single equation for the whole sampled surface, it cannot have the same precision that the kriging local estimation method may have.

Standard deviation of the estimation error (*fig.* 6b) is a function of spatial distribution of data values within the range of the variogram with respect to point where estimation is to be done. This error term is also dependent on the nugget variance and the number of points involved in the interpolation (neighbours) but independent on the observed values themselves. It usually increases at the edges of the kriged area (*fig.* 6b) because there are fewer data points involved in the estimation. If these values have to be as reliable as those of the centre of the kriged surface, sampling scheme should be extended beyond the boundaries of the area to be mapped.

CONCLUSION

Conventional methods of spatial structure analysis of soil organisms generally use diverse indices based on sample mean and variance. Even if some of them give a satisfactory quantitative measurement of the amount of aggregation, they do not allow to investigate the true pattern within the sampled area. This task is achieved by geostatistical analysis. The variogram analysis allows to determine whether the variable is autocorrelated or not. If a spatial structure is present, kriging procedure can be used to estimate values at unsampled points together with their associated estimation error. Estimates can be used to draw both contour maps of the variable and maps of the estimation error. In addition, the cross semi-variance analysis constitutes a way to investigate relationships between spatially structured variables.

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