GEOSTATISTICAL MODELS FOR AIR POLLUTION

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Abstract

The objective of this paper is to present geostatistical models applied to the spatial characterisation of air pollution phenomena. A concise presentation of the geostatistical methodologies is illustrated with practical examples. The case study was conducted in an underground copper-mine located on the southern of Portugal, where a biomonitoring program using lichens has been implemented. Given the characteristics of lichens as indicators of air pollution it was possible to gather a great amount of data in space, which enabled the development and application of geostatistical methodologies. The advantages of using geostatistical models compared with deterministic models, as environmental control tools, are highlighted.

1. INTRODUCTION

Air quality modelling is an essential tool for most air pollution studies. Monitoring data are indispensable for inferring theories or parameters and calibrating or validating computer simulation packages. However, only a well-tested simulation model can be a good representation of the real world, its dynamics and its responses to perturbations. The monitoring design and activities should be integrated with numerical models in order to avoid investments and efforts to collect data that remain unused or even turn out useless.

Hence, air quality modelling is an indispensable tool for prevention and control of air pollution [1], covering the following tasks:

- planning the control of air pollution episodes;
- selecting locations of future sources of pollutants, in order to minimise their environmental impacts;
- assessing responsibility for existing air pollution levels;
- establishing emission control strategies;
- evaluating proposed emission control techniques and strategies.

Air quality models can be divided into physical and mathematical models. The physical models consist on small-scale laboratory prototypes that try to reproduce the real phenomena. The mathematical models are a set of analytical or numerical algorithms that describe chemical and physical processes. Often, the data obtained through physical models may be very useful for understanding the processes and helping the developers of mathematical models. Mathematical models can be subdivided into deterministic and statistical models. A general distinction between deterministic and statistical approaches in air pollution is that deterministic models concept are based on physical principles, while statistical models are characterised by their direct use of air quality measurements to infer statistical relationships. Nevertheless, some deterministic models are based on statistical diffusion theories.

In the category of statistical models are included a large set of approaches namely time series analysis, Kalman filters, receptor modelling techniques and interpolation algorithms. In the last years, the number of applications using geostatistical models applied environmental sciences have been increasing with successful results on modelling soil [2, 3], water [4, 5] and air pollution [6–9].

Geostatistics offers a way of describing the spatial continuity that is an essential feature of many natural phenomena [10]. In the former years, geostatistics was used mainly as an interpolation technique, which took advantage of the ability to incorporate spatial continuity. More recently geostatistical models for the uncertainty assessment have been developed and applied to environment sciences in particular for the polluted sites characterisation. Such models based on the indicator formalism allow the risk evaluation related with the impact of the pollutant [11, 12].

Two practical examples illustrate these geostatistical methodologies. This case study was conducted in an underground copper mine where a biomonitoring programme with lichens has been implemented.

2. BIOMONITORING PROGRAMME

The study was conducted in the area of influence of a large industrial facility that produces copper concentrates from ore, located in southern Portugal. The main air pollution source at mine site is fugitive dust emissions from the concentrate stockpiles with high copper grade and a particle size of about 20 μm.

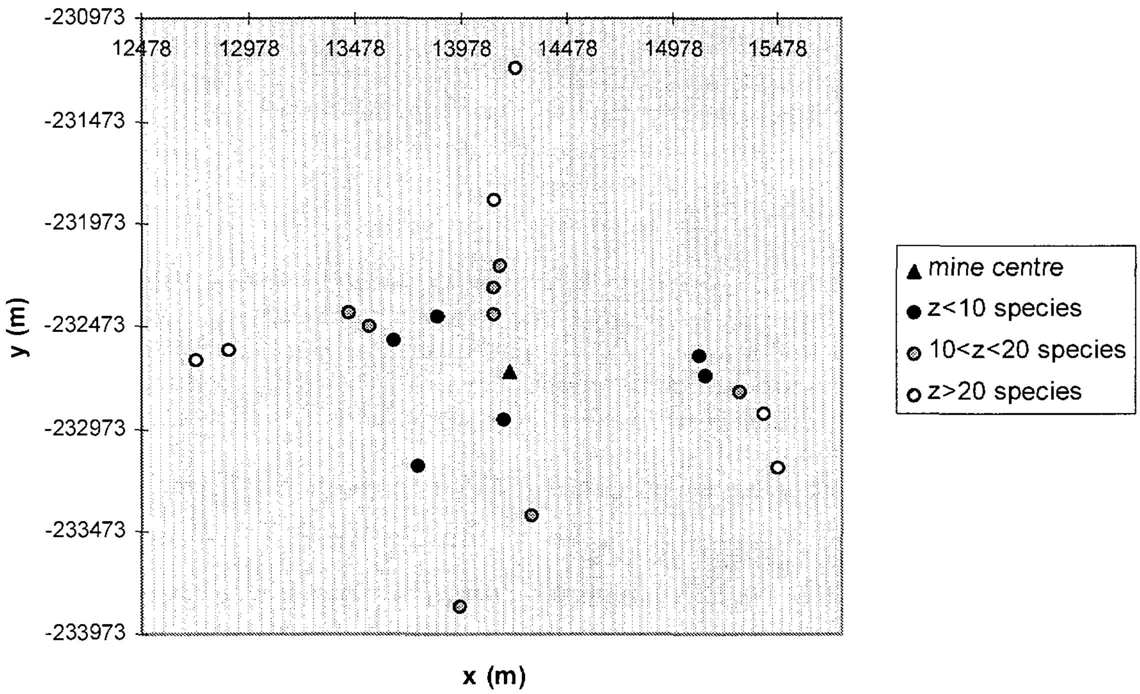

Figure 1. Studied area around the mine site and sampling locations.

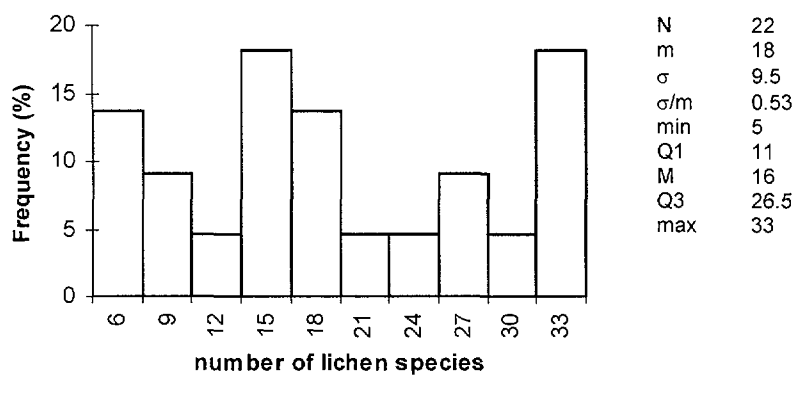

Figure 2. Histogram and basic statistics of the studied variable (number of lichen species).

Epiphytic lichens show differential sensitivities to air pollution, i.e., the most sensitive lichens tend to disappear from polluted areas whereas the more tolerant species can be seen in areas with moderate pollution emissions [13, 14, 15]. Moreover, since lichens are slow-growing organisms they may be used as long-term integrators of environmental conditions. Because species loss occurs in areas with heavy air pollution, in this work the number of epiphytic lichen species was used, as a direct measure of biodiversity, to evaluate the impact of the copper mine on lichen flora [16]. The lichen biodiversity study consisted in recording at each sampling point the number of epiphytic lichen species from 6-10 Quercus ilex trees and exceptionally from Olea europeae. The sampling was conducted according the pattern shown in Figure 1, in 1993.

The number of lichen species varies from 5 at the centre of the mine (near the stockpile location) to 20-30 species at 2 km from the mine (Figure 2). A detailed study description about the biodiversity can be found in [17, 18].

The relationship between the number of lichen species and their thallus growth forms with distance from the centre of mine confirms that the main source pollution was focused on the centre of mine site [18].

3. GEOSTATISTICS

3.1 Spatial dispersion of lichens

The main geostatistical tool for the spatial continuity characterization of a given attribute is the spatial covariance or the variogram [10]. In fact, spatial features of the attribute like preferential patterns of continuity (anisotropic behaviour), spatial dispersion at diferent scales, etc., can be visualised and quantified by the variogram. In Figure 3, one can see the variogram of the number of lichens species. Two discontinuities reveal two structures at different scales. Up to 400 m from the mine site (1st structure) only crustose lichens occur given their robustness to adverse conditions. Foliose lichens and some fruticose lichens only appear at distances beyond 400 m. More fruticose lichens, such as usnea species, occur beyond the 1200 m (2nd structure).

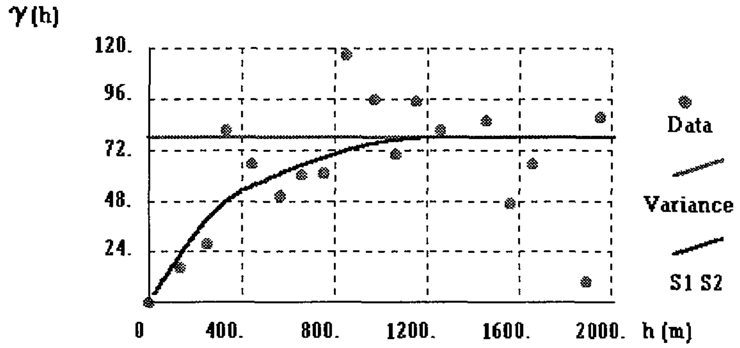

Figure 3. Semi-variogram of the number of lichen species and theoretical model fitted.

The variogram was modelled by a sum of two spherical structures:

$$\gamma(h) = Sph_1(a_1 = 400, c_1 = 50) + Sph_2(a_2 = 1200, c_2 = 40.25)$$

3.2 Estimation of main attribute

The number of lichens was estimated by Kriging in a regular grid of points covering the entire area around the mine, shown in Figure 4.

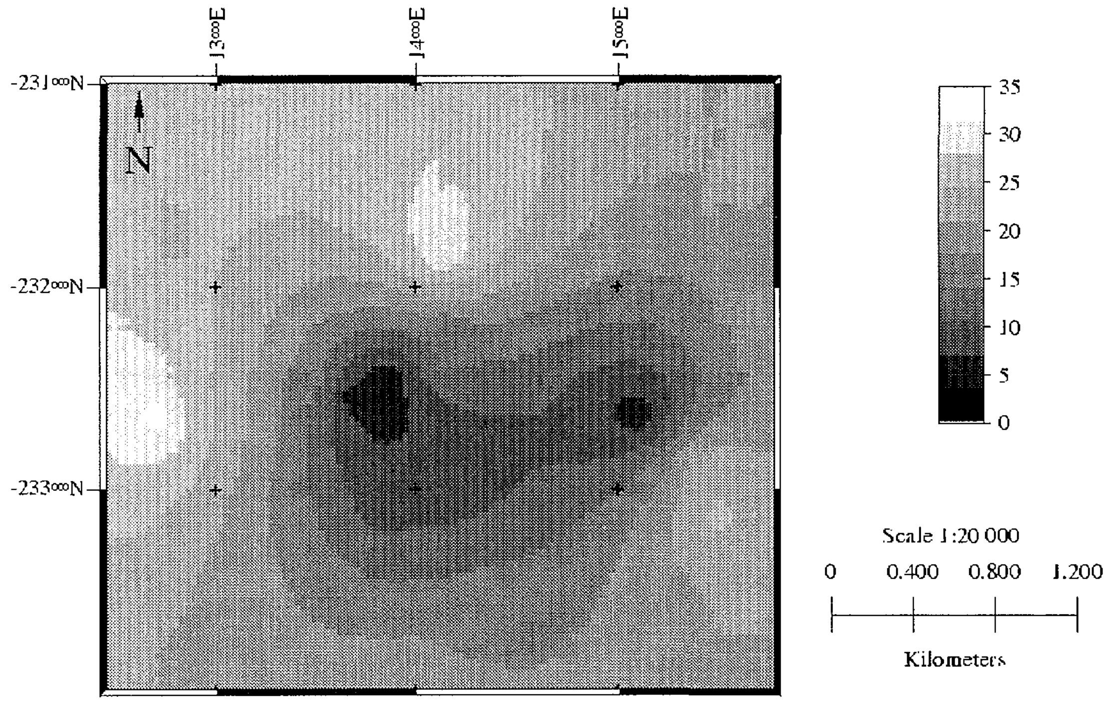

Figure 4. Estimated map representing the number of lichen species around the main mine site.

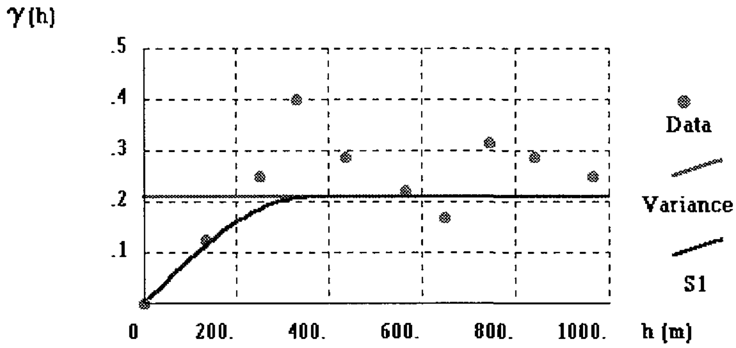

Figure 5. Experimental indicator variogram and theoretical model fitted:
$C_0 = 0$, $C_1 = 0.21$, $a_1=350$ m.

3.3 Uncertainty assessment with indicator formalism

With these models one intend to assess the uncertainty about the unknown, rather than calculating the best estimator of it. In fact, the objective is to estimate the probability of the main attribute $Z(x_0)$ to be lower than a threshold z at a given location x_0, given the sample values $Z(x_\alpha)$, α=1, N:

$$\Pr ob\ \{Z(x_0) < z \mid Z(x_\alpha),\ \alpha = 1, N\}$$

Different geostatistical models can be used for the estimation of local conditional distribution functions [11, 19]. To estimate these local conditional probabilities one has used the indicator formalism. An indicator variable is obtained through a binary transform of the original variable Z(x) with a threshold z.

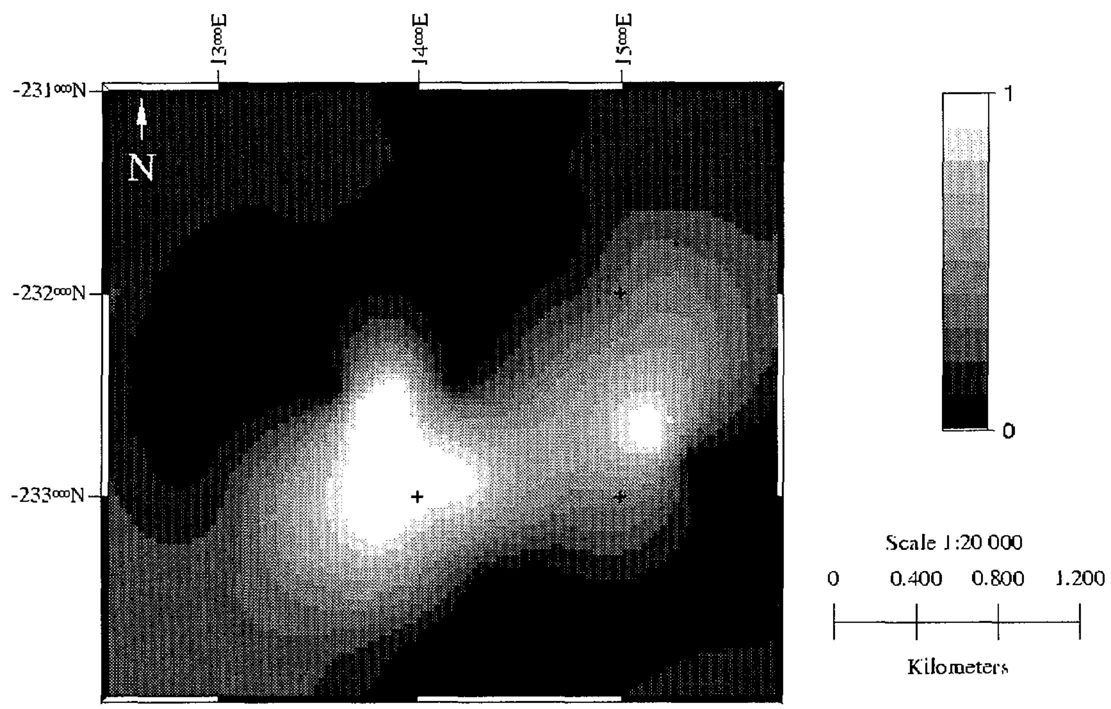

Figure 6. Probability map of occurring less than 10 lichen species.

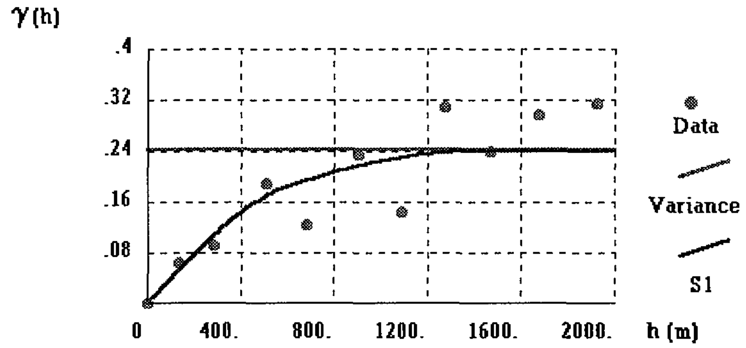

Figure 7. Experimental indicator variogram and theoretical model fitted: $C_0 = 0$, $C_1 = 0.15$, $a_1 = 600$ m.; $C_2 = 0.09$, $a_2 = 1400$ m.

$$I_z(x) = \begin{cases} 1 & \text{if } z(x) < z \\ 0 & \text{otherwise} \end{cases}$$

In the sample locations, $I(x_\alpha)$, $\alpha = 1, \ldots N$ has the meaning of the probability of sample x_α to not exceed the threshold z:

$$I(x_\alpha) = prob\{z(x_\alpha) < z\}$$

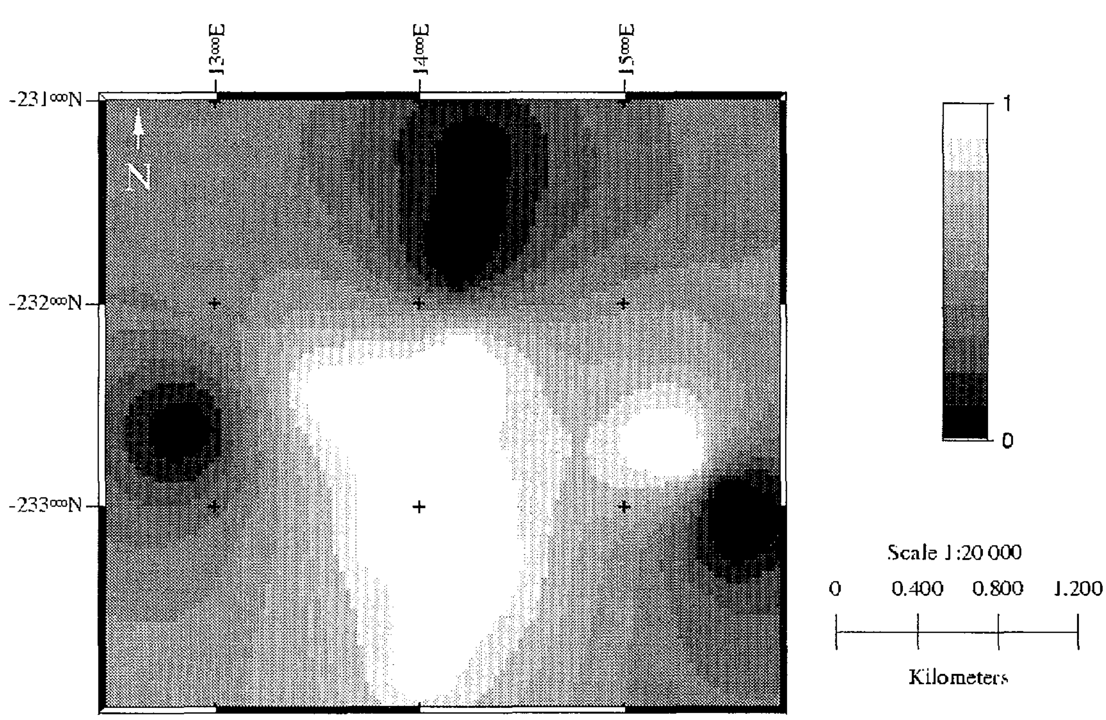

Figure 8. Probability map of occurring less than 20 lichen species.

The indicator Kriging of any point x_0 is an estimator of the local conditional probability of x_0 to exceed z.

$$[I(x_\alpha)]^* = \sum_{\alpha} \lambda_\alpha I(x_\alpha) = [prob\{z(x_0) < z \mid (I(x_\alpha), \alpha = 1, N\}]$$

In the present case study one intend to calculate, just for illustrative purposes, the areas below and above the threshold 10 and 20 (number of identified lichen species).

3.3.1 Threshold of 10 lichen species

For the threshold 10 (lichen species) the following indicator variable was defined at experimental sampling points (see Figure 1):

$$I_z(x) = \begin{cases} 1 & if \quad Z(x) \leq 10 \\ 0 & if \quad Z(x) > 10 \end{cases}$$

The indicator values have the following statistics:

$$m_{I10} = 0.30 \qquad \sigma_{I10}^2 = 0.21$$

The calculated omnidirectional variogram (see Figure 5) reflects basically the shape of the affected vegetation coverage around the mine site. A spherical model with 350 m of range and null nugget effect was fitted to the experimental variogram.

Figure 6 represents the map of probabilities of occurring less than 10 lichen species. The uncertainty related with the impact of dust emissions around the mine can be visualised with this map or other identical maps using different thresholds.

3.3.2 Threshold of 20 lichen species

For the threshold 20 (lichen species) the following indicator variable was defined at experimental sampling points (see Figure 1):

$$I_z(x)=\begin{cases}1 & \text{if } Z(x)\leq 20\\ 0 & \text{if } Z(x)>20\end{cases}$$

The indicator values have the following statistics:

$$m_{I20} = 0.64 \qquad \sigma_{I20}^2 = 0.24$$

A sum of two spherical models with respectively 600 m and 1400 m of range and null nugget effect was used to fit the experimental omnidirectional variogram (see Figure 7).

Figure 8 represents the map of probabilities of occurring less than 20 lichen species.

4. CONCLUSIONS

The lichen biodiversity sampling enabled the development and application of geostatistical methodologies to spatially characterise the air quality. It is important to remark, however, that lichens are slow growing organisms and they must be used only as long term integrators of the environmental conditions.

Output maps of estimated number of lichen species represent the average air quality during a long period of time. Maps of estimated probabilities of occurring less than a certain number of species (i.e., a given threshold) represent the uncertainty related with the impact of dust emissions around the mine.

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