Proceedings of ECOpole

Vol. 2, No. 1 2008

Jarosław ZAWADZKI¹ and PIOTR FABIJAŃCZYK¹

GEOSTATISTICAL ASSESSMENT OF ANTHROPOGENIC SOIL CONTAMINATION USING MAGNETOMETRIC MEASUREMENTS

GEOSTATYSTYCZNE SZACOWANIE ZANIECZYSZCZENIA GLEB ZA POMOCĄ POMIARÓW MAGNETOMETRYCZNYCH

Summary: The potential soil contamination with heavy metals can be assessed using geochemical analysis. Apart from these expensive and time consuming methods, some rapid, simple and cheap geophysical methods can be used. One of these methods is field magnetometry. Magnetic susceptibility is a convenient measure of determining the concentration of ferrimagnetic particles that serve as carriers of various pollutants such as heavy metals by rapid and non-destructive means. However, because of complex correlations between magnetic susceptibility and soil pollution, the field magnetometry cannot be considered as the universal method of soil pollution investigation. For each new area of investigation, the results should be reinterpreted taking into account not only the type of pollution but also many pedogenic, biogenic and environmental factors. In practice, it is very difficult to measure and consider all these factors. This is why a further improvement of the magnetometric method is necessary to allow the technique to be used as a quantitative tool for soil pollution investigations. In particular, the interpretation of results should be improved. Geostatistical methods, which are focused on the spatial variability of a studied phenomenon, are an effective tool for field magnetometry applications and interpretation of its results. This paper describes the role of the geostatistical methods in the standardization of field magnetometry. Different measurement and geostatistical modeling strategies are presented, compared and discussed. The paper includes also a case study in which the geostatistical contribution to standardization of the magnetometric method is thoroughly demonstrated. Moreover, the paper discusses practical aspects of geostatistical standardization of magnetometric methods to allow for easy use them during surveys.

Keywords: field magnetometry, soil pollution, topsoil magnetic susceptibility, anthropogenic pollution, geostatistics, data integration, standardization

Geostatistics offers many tools for the analysis of spatially correlated data and is well-suited to the study of natural phenomena. Formerly, geostatistics was developed for the mining and petroleum exploration industries [1, 2]. However, due to many advantages of these methods, they are also applied in other branches. The main goals of geostatistics are describing and analyzing spatial variability using different measures of spatial variability [3-5]. The majority of classical statistics do not utilize the spatial information, which is a natural characteristic of environmental data. According to this geostatistics has many improvements and advantages over classic statistics, which enables to precise and effective analyses of results of field measurements concerning soil pollution.

Magnetic susceptibility is one of the soil properties, which enables to assess the extent of soil contamination with heavy metals [6]. The development of field magnetometry resulted from a need for fast and cheap methods for the detection of industrial pollution of soil. Recently, these measurements became recognized as a useful and effective method for detecting the presence of different heavy metals in soil. Magnetic susceptibility of top soil layers is often strongly affected by dust deposition of anthropogenic origin at the soil surface, which is a source of many magnetic particles, and amongst them heavy metals. An increasing number of studies were carried out using magnetometry to assess the soil

¹ Department of Informatics and Environment Quality Research, Warsaw University of Technology, Nowowiejska 20, 00-661 Warszawa, email: j.j.zawadzki@gmail.com, piotr.fabijanczyk@is.pw.edu.pl
contamination with heavy metals [7-9]. Significant positive correlations were found between the magnetic susceptibility and the content of heavy metals of anthropogenic origin in soil [10-12]. Due to these correlations, it is possible to estimate the extent of areas with heightened values of soil magnetic susceptibility, and simultaneously potentially polluted with magnetic compounds and accompanying heavy metals. Consequently, fast and cheap field magnetometric measurements can supplement or, in some specific situations, completely replace the chemical analyses.

Geostatistical methods

One of the central tools of geostatistics is the semivariogram function, which plot is commonly called a semivariogram [13]. This measure is used to analyze spatial continuity of phenomena. The application of the semivariogram requires that the data meet the intrinsic hypothesis for a regionalized variable. Semivariance can be calculated separately for different directions, which produce anisotropic semivariance or combined to produce an omnidirectional semivariance. The experimental semivariance is calculated as one-half of the average squared difference in data values for every pair of data locations separated by a vector. These values are then plotted against the distances between data pairs - the h vector. The following formula is used for the semivariance calculations:

$$\gamma(h) = \frac{1}{2N} \sum_{i=1}^{N} [Z(x_i) - Z(x_i + h)]^2$$

where: $x_i$ - a data location, $h$ - a lag vector, $Z(x_i)$ - the data value at location $x_i$, and $N$ - the number of data pairs spaced a distance and direction $h$ units apart. A frequent form of the experimental semivariogram and its model is shown in Figure 1.

![Fig. 1. A common semivariogram form](image)

The obtained experimental semivariogram is used to fit an appropriate theoretical model, such as the spherical or exponential. The model of experimental semivariance is characterized by some parameters. The sill is the semivariance value at which the semivariogram reaches the plateau. The range, often called a range of influence or
correlation, is the distance at which correlations amongst data is no longer exists. The nugget effect represents the vertical discontinuity at the origin, and is a combination of sampling error and short-scale variation that occurs at a scale smaller than the closest sample spacing. In the most cases, the semivariogram is modeled using linear combination of few basic models, which combination is often referred as “nested structure”.

Other important measure of spatial correlation used in cokriging is the cross-semivariogram, which is calculated for two variables, like in case of semivariogram. The following formula is used for the cross-semivariance calculations

$$\gamma_{wz}(h) = \frac{1}{2N} \sum_{i=1}^{N} [W(x_i) - W(x_i + h)][Z(x_i) - Z(x_i + h)]$$

where: $x_i$ - a data location, $h$ - a lag vector, $Z(x_i)$ and $W(x_i)$ - the data values at location $x_i$ of different quantities, and $N$ - the number of different type data pairs separated by length of the vector $h$.

The cross-semivariogram quantifies the cross-correlations between two different variables, where one is called primary and second one additionally variable. In some cases, when only small data sets are available simpler and easier to calculate measure of spatial variability is calculated - the pseudo-cross-semivariogram:

$$\gamma_{_{wz}}(h) = \frac{1}{2N} \sum_{i=1}^{N} [Z(x_i) - W(x_i + h)]^2$$

The possibility of calculating and modeling the reliable semivariogram is a crucial for application of some geostatistical methods.

One of the most common geostatistical method of spatial estimation is kriging, which produces estimates $Z^*$ with minimum-variance taking into account the spatial variability characterized by the semivariogram.

$$Z^* = \sum_{i=1}^{n} \lambda_i z_i$$

where: $\lambda_i$ - the weights, $z_i$ - the known data values.

The kriging weights are computed by minimizing the estimation variance allowing for the non-bias condition. Among many different types of kriging, the most popular are ordinary kriging, simple kriging which assumes that the mean value to be known, universal kriging (with the trend model), block kriging, which is used when point measurements are available, but the study requires the calculation of the aerial value over a larger domain. Other important kind of kriging is indicator one. In this procedure, after transforming the original values into indicator values, the probability maps of non-exceeding some critical threshold are calculated.

Cokriging is a variety of kriging, which allows using multiple variables, correlated with each other. This method is useful when measurements of primary variable are difficult to perform, too expensive or too rarely sampled. In such situation it is possible to integrate different additional data, eg biological or chemical with physical ones, current with historical ones, remote observations with field measurements. This is done due to cross-correlations between primary and secondary variables. Similarly to kriging, cokriging minimizes variance of estimation error of primary variable, utilizing cross-correlations
between primary variable and secondary variables. The value estimated at unknown location, is calculated using linear combination of both variables:

\[
Z^*(x_0) = \sum_{k=1}^{N_1} a_k z(x_k) + \sum_{i=1}^{N_2} b_i w(x_i)
\]

where: \( Z^*(x_0) \) - the prediction at location \( x_0 \), \( z(x_j) \) - the \( j^{th} \) nearby sample primary value weighted by \( a_j \), and \( z(x_l) \) - the \( l^{th} \) nearby secondary value weighted by \( b_l \). \( N_1 \) and \( N_2 \) - respectively, the numbers of nearby sample primary values and nearby secondary values.

Application of cokriging demands semivariogram models for primary and secondary variables as well as cross-semivariances to be known and modeled. The cokriging system has a unique solution with positive cokriging variance when the so-called the linear model of coregionalization (LMC) occurs.

Cokriging usually gives much better spatial precision of estimation than kriging, with smaller error variance, when primary variable is strong enough correlated with secondary ones. The values of classical Pearson correlation coefficient should be greater than 0.4 and less than ca 0.9. In case of weak correlations (value less than 0.4) estimation is not improved but even results are worse in comparison with kriging. When Pearson correlation coefficient is close to 1.0 the multivariate linear regression technique gives the similar results as cokriging with considerable less effort. Apart from classical correlations also spatial ones are used in cokriging. Accordingly not only high value of the Pearson coefficient is needed but first of all well-developed cross-semivariances with large enough ranges of influence and small enough nugget to sill ratio.

In some cases the application of cokriging can be difficult. When only small data set of primary variable is available it may be very hard to calculate the reliable cross-semivariograms. Apart from small data sets problem, very often primary variable is sampled using clustered and irregular sampling grids. Such situation can also make the cross-semivariogram calculation more difficult. In such situation it is necessary to use different method of data integration.

One of them is Co_Est method [14]. The technique transforms the secondary dataset into the primary one using the so-called pedotransfer functions (PF), which often are described by regression equations. The result of transformation is a larger data set of primary variable, which can be subsequently used in different geostatistical procedures using only one semivariance, like eg kriging.

Another approach is to replace the cross-semivariance with some robust estimators. One of them are pseudo-cross-semivariances [15, 16]. This kind of cokriging do not need that both variables are measured at the same location. This characteristic is very important particularly for soil pollution studies when fast screening methods like filed magnetometry is used. In addition, a smaller amount of data is needed for the calculation of pseudo-cross-semivariograms, which are more resistant to outliers than cross-semivariances.

The ordinary cokriging is only basic kind of cokriging method. Similarly like in case of kriging, also indicator variant of cokriging can be used. This technique uses indicator values of both primary and secondary variables. As a result of estimation, maps of probability of not exceeding some critical thresholds are calculated. This method is also very resistant to outliers, and is appropriate for non-Gaussian distributions. Unfortunately at the same time it requires the calculations and modeling auto and cross-semivariances for
many thresholds, which may be time-consuming. One more advantage is the possibility to comprise also qualitative information of various types by appropriate coding this information. Accordingly it is possible to take into account common environmental qualitative data as eg rock or soil type, land use, which may be advantageous particularly in field magnetometry.

**Applications of geostatistics in field magnetometry**

In field magnetometry a few types of measurement can be performed. The most common types are the surface measurement (usually carried out with MS2D Bartington sensor), and measurement of soil magnetic susceptibility in soil profile (usually carried out with SM400 sensor). The penetration range of MS2D sensor is about 10 cm, and accordingly measurement done with this sensor gives as a result a averaged soil magnetic susceptibility from depth from 0 to 10 cm [17, 18]. The measurement in soil profile gives as a result a plot of magnetic susceptibility against the depth (compare with Fig. 2). It is more precise measurement in comparison with the surface one, but it is also more time-consuming one. Results of these two types of measurements can be analyzed separately, however using geostatistical integration of data the analyses may be more precise.

The magnetic susceptibility usually shows characteristic distribution in the soil profile. Very frequently peak value is observed at the depth of several cm, which is directly connected with the thickness of the soil organic horizon. The previous studies confirmed significant positive correlation between the magnetic susceptibility in soil profile and the content of heavy metals. On areas where the organic horizon is well-developed the anthropogenic magnetic particles are typically concentrated in fermentation and humic subhorizons.

![Fig. 2. Distribution of magnetic susceptibility in soil profile](image_url)

Usually the significant correlation exists between surface and vertical measurements. Accordingly, cokriging and Co_Est methods can be applied in order to integrate these
measurements. The selection of one of above-mentioned methods depends on the several factors, like number of samples, and sampling grid density and geometry, which influence the possibility of modeling the spatial variability and semivariograms.

Magnetometric measurements can also effectively supplement chemical analyses of heavy metal content in soil, though magnetometry can not completely replace the geochemical methods. Accordingly, there is a need for integration of both chemical and magnetometric measurements. Geostatistical methods like cokriging and Co_Est method enable effective integration of these types of measurements. It is possible to perform magnetometric measurements in few stages (Fig. 3). Firstly, study area can be sampled with relatively sparse sampling grid of surface soil magnetic susceptibility measurements, dense enough to calculate initial semivariogram. After that the spatial distribution of magnetic susceptibility can be obtained using ordinary kriging. Analysis of this distribution can reveal the areas with heightened magnetic susceptibility and simultaneously potentially contaminated with heavy metals. After that, additional surface measurements can be
performed and also measurements of magnetic susceptibility in soil profile. Vertical measurements are more resistant to many environmental factors, which can affect the surface measurements, like soil type, forest bedding thickness etc. After this second stage of measurements, the precision of previously obtained spatial distribution of soil magnetic susceptibility can be improved. Furthermore, at this stage data integration methods can be applied to integrate the surface and vertical measurements to maximize the amount of information collected in the file during the measurements. Moreover, indicator methods can be applied to calculate probability maps of exceeding some critical threshold of soil magnetic susceptibility, which denotes the potential soil contamination with heavy metals. After that the locations of chemical samples can be determined in more precise way. After sampling the study area with chemical samples, geostatistical methods can be applied both to integrate the chemical and magnetometric measurements and to calculate the probability maps of potential soil contamination with heavy metals.

Conclusions

Use of geostatistics in field magnetometry can be advantageous beginning from planning the measurements, through analyzing the results of measuring surveys and concluding about potential soil contamination.

Combining the filed magnetometry and chemical analyses with geostatistical methods enables to better plan the measuring survey. It is possible to better analyze the spatial variability of studied phenomenon, using proper sampling density or to perform multistage measurements. It is also possible to place samples in the way, which minimizes possible sampling errors and simultaneously maximizes the amount of information collected in the field.

It is also allowed for integration different types of magnetometric measurements, which can be carried out in the field ie measurements of magnetic susceptibility in soil profile and surface measurements of magnetic susceptibility. Integration of chemical and magnetometric measurements using geostatistical methods allows often overcoming problems connected with small data sets or irregular sampling designs.

Accordingly, use of geostatistical methods enables to obtain more precise spatial distributions of heavy metals content in soil greatly reducing ecological risk or measurement costs.

Acknowledgements

The study was granted by the Ministry of Sciences and Higher Education in the frame of Project no 3 T09D 01328.

References

GEOSTATYSTYCZNE SZACOWANIE ZANIECZYSZCZENIA GLEB ZA POMOCĄ POMIARÓW MAGNETOMETRYCZNYCH


Słowa kluczowe: magnetometria terenowa, zanieczyszczenie gleb, podatność magnetyczna, zanieczyszczenie antropogenne, geostatystyka, integracja danych, standaryzacja