

Methods for geochemical anomaly separation:
the geostatistical and multifractal approaches

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Abstract

Separation of geochemical anomalies from background has always been a major concern of exploration geochemistry. The search for methods that can make this analysis quantitative and objective aims not only at the reduction of subjectiveness but also at providing an automatic routine in exploration, assisting the interpretation and production of geochemical maps. This report discusses two methodologies which aim at the same objective of geochemistry anomaly separation: multifractal theory and geostatistics. Geostatistics is a powerful tool for the analysis of regionalized variables, and factorial kriging has been successfully applied to map different components of a random function in a domain. These components, in geochemical analysis, correspond to the different average grades in an area, each one related to a given geological structure responsible for the phenomenon. This same problem has also been approached in a different manner, by means of multifractal modeling. At the present time, a proposed multifractal model is the only ones which aims at giving quantitative values for the anomalous thresholds by means of the relations between areas enclosing a given concentration and concentrations. This model relies on the assumption that the collection of geochemical values follow a multifractal model, *i.e.* the measured concentrations in a given area are self-similar at any scale. It is also discussed, in relation to the multifractal model, how to prove if a given data set is multifractal or not. However, it has been shown that the model is efficient even if such proof fails, which opens a series of questions regarding the true multifractal nature of the model. It is briefly discussed that some measurements still need the geostatistical framework in order to be representative and robust, and a comparative study should be performed between multifractal models and factorial kriging. Since it is not proved that the multifractal model is universal, although it is extremely simple to implement and can give very quick results, its combination with factorial kriging could give a very powerful and robust method used in geochemical exploration.

1. INTRODUCTION

The definition of geochemical anomalies from background in areas where the concentration of elements reveal a potential economic interest is a major objective in the analysis and interpretation of geochemical data. Some of the methods proposed comprise empirical models, others come from the developments of theoretical geostatistics, and from the theory of multifractals. The objective of this technical report is to present some of these methods, and discuss the way they may be applied to geochemical data.

Different types of substances can be analyzed in a given area in order to evaluate its geochemical interest. These may be rock samples, soil samples, ground and surface waters, mineral concentrates and stream sediments. Depending on the type of sampling performed, so too the analysis of the results must be different. The methods here described can be applied to any of this kind of sample sets, although this report will focus only in applications to soil sampling analysis. Soil samples show a multitude of chemical elements that can be explained as contributions from different source rocks. As a matter of fact, it is virtually impossible to fully separate which amount of a given element concentration is due to a particular rock type (mixtures are obviously expected). Soils may also be subjected to motion from one location to another, giving rise to geochemical dispersion haloes rather than anomalous spots (or more circumscribed areas with anomalous values) as it would be expected if the rock was analyzed instead. So, one important thing when such analyses are performed is to have quantitative information about the chemical nature of the different rocks appearing in an area which is about to be explored. Other parameters such as the thickness of the soil, local drainage, topography and geological structural features are very important to be able to make a correct interpretation of the obtained results. If any of these parameters is not properly evaluated, severe risks occur of misunderstanding some of the results and of incorrect interpretation of the data.

The development to follow does not explore very much the problem of dealing correctly with the sample set. This problem is extensively treated in several

books on statistics and geostatistics however, part of it must also come from the researcher's own feeling for the problem to study. It will be discussed in a very broad sense some applications already made using geostatistics and multifractal modeling as approaches to the problem. The ultimate goal shall be to establish a comparative study of both methodologies in order to infer their applicability and advantages of use.

2. MODELS FOR GEOCHEMICAL ANOMALY SEPARATION

The approaches to the separation of geochemical anomalies from background values has deserved attention for a long time, and methods such as moving averages, kriging and probability plots have been used to deal with this problem. The concern here is to introduce two important methodologies used to define a geochemical anomaly: geostatistics and multifractal theory. Both of these methodologies have been used but there is not much cross-reference of data from other sources that could be taken as a validation criteria of the results obtained, especially when one deals with soil geochemistry given the problems it may rise in the interpretation of the results. It is worth noting as well that no work has been done yet comparing the different approaches. This is a very important remark since the different methodologies require that the data set should be analyzed differently and the amount of time needed to do it is different as well. This obviously depends on the objective underlying the study, however it may be apparent that a given methodology is accessible and easily implemented just to give some quick results.

The work of Cheng *et al.* [3] has shown how geochemical data sets can be modeled and treated as distributions that follow a multifractal model. The model proposed is indeed very simple and straightforward, which puts it in a very privileged situation as a potential tool for a rapid analysis of geochemical anomalies. The basic principle of this approach relies on the observation of the way areas (defined by contour lines) enclosing values greater than a given grade vary as the grade is changed. In general, if $A(\rho)$ is the area enclosing values greater than the concentration value ρ defined by the contour line, and if ν represents the threshold of the anomaly, the following empirical model holds:

$$A(\rho \leq \nu) \propto \rho^{-\alpha_1} \tag{2.1}$$

and

$$A(\rho > \nu) \propto \rho^{-\alpha_2}. \tag{2.2}$$

In these equations α_1 and α_2 are constants, and it is immediately evident that in a log-log plot the relation between area and concentration gives two straight lines with slopes α_1 and α_2 . The point where the slope changes is coincident with the value of $\rho = \nu$, which must satisfy both equations simultaneously (considering that equations 2.1 and 2.2 form a continuous function, so that ν is a point belonging to both). These same authors [3] have demonstrated that, if the element concentration per unit area satisfies a fractal or multifractal model, then $A(\rho)$ has a power-law type relation with ρ . For a range of ρ close to its minimum value, ρ_{\min} , the predicted multifractal power-law relations are:

$$A(\rho) = C_1\rho^{-\alpha_1} \quad (2.3)$$

and

$$A(T) - A(\rho) = C\rho^\beta, \quad (2.4)$$

where $A(T)$ represents the total area, C_1 and C are constants, and α_1 and β are exponents associated with the maximum singularity exponent. For a range of ρ close to its maximum value, ρ_{\max} , the predicted power-law relation is simply

$$A(\rho) = C_2\rho^{-\alpha_2}, \quad (2.5)$$

where C_2 is a constant and α_2 is the exponent associated with the minimum singularity exponent.

Although these models may describe a geochemical data set, they not necessarily mean that such data set shows a multifractal distribution. However, appropriate measurements can be performed in the data in order to test the multifractal hypothesis [6], which will be object of discussion later on. This question is actually a very striking one, since this model has already been successfully applied to data sets that fail to comply to the multifractal hypothesis. This will be an issue for further discussion.

Besides the paper of Cheng *et al.* [3] this model has not deserved very much attention yet. Subsequent works [7, 8] have applied the method successfully to data sets for the definition of anomalies in areas with potential gold mineralizations and also to chromium-nickel and vanadium mineralizations in basic and ultrabasic rocks, respectively. Another paper [5] presents a different method of separation of geochemical anomalies, minimizing misclassification of anomalous and background samples using a moving average technique on a new spatial statistical approach, which give a good agreement with the results of the multifractal model.

The geostatistical approach is based in the identification of different spatial structures evidenced by data at different scales. The experimental variogram is the basic tool to model the correlation between sample points as a function of distance within the geostatistical framework. Factorial kriging is a theoretical development due to Matheron [15] in which kriging is presented as a tool to map the different structures of a given random function or, in a complementary way, to filter some of these structures. These structures, in soil geochemistry, may be viewed as the background and anomalous concentrations displayed by a set of samples in a given region. The approach may be univariate or multivariate (if more than one chemical element is important to the characterization of a given area). Matheron [15] presents the problem by decomposing a random function in a series of uncorrelated factors which in turn are linearly estimated using the appropriate set of kriging equations. The application of factorial kriging, like geostatistics in general, largely surpass the aims of geochemistry and mining, and several papers show the application of this method to ground and surface waters as well as to soil geochemistry [16, 9, 12, 17].

The sections to follow will discuss shortly the fundamentals of the theory behind each presented approach. As a final statement some reasons will be advanced for the need to undertake a comparative study between them.

3. THE GEOSTATISTICAL FRAMEWORK

Geostatistics has been the most widely used method for the analysis of spatial data, ever since its first applications to mining. The purpose of this introduction is not to give a full account of the geostatistical theory, but only a very general and fundamental description of its theoretical basis, necessary to justify what is developed in the sections ahead. The reader should be referred to some reference books [11, 13, 18], in which the presentation below is based. A most interesting paper of Matheron [14] is also worth noting since it presents, in a very concise way, the theory of regionalized variables by the time mining was the main (and only) application of geostatistics.

Considering a domain D , we call *regionalized variable* to the associated function $z(x)$ of $x \in D$, which can be viewed as a draw from an infinite set of random variables. This set of random variables are realizations of the *random function*, $Z(x)$, in the domain. Therefore, an observation at any location x_α , $z(x_\alpha)$ with $\alpha = 1, \dots, n$, is considered as an outcome of a random mechanism. Because the underlying physical principle is in general very complex, its results are treated in a probabilistic way and it is within this framework geostatistics is developed.

In order to simplify the problem, some assumptions must be considered such as strict stationarity. This property implies that the random function stays the same when a translation operation is performed on any set of n of its points, regardless of the translation vector h . However, in geostatistics, random functions are assumed to be *second-order stationary* in most of the cases. This implies that the random function has a mean which is the same everywhere in the domain D , and the variance between any two pairs of samples is a function of their distance (h) alone.

The ultimate goal is to be able to estimate the variable value at a given point from a finite number of observations. The variable at location x_0 may be linearly estimated from known data points in the domain D according to the equation

$$z^*(x_0) = \sum_{\alpha=1}^n w_\alpha z(x_\alpha), \quad (3.1)$$

where w_α are the weights assigned to each known value $z(x_\alpha)$.

In geochemical analysis, samples always show some degree of spatial correlation, and the calculation of the experimental variogram allows to model the sample correlation for any vector separation h . Therefore, for any pair of sampled points (observations) in the domain D , far apart from each other of a quantity h , the computed experimental variogram is

$$\gamma^*(h) = \frac{1}{2n} \sum_{\alpha=1}^n (z(x_\alpha) - z(x_\alpha + h))^2. \quad (3.2)$$

This experimental variogram is then substituted by the theoretical variogram function to ensure that the variance of any linear combination of sample values is positive. This is guaranteed by the use of *positive definite* variogram functions [11, 18].

Another way of dealing with the problem is using a covariance function $C(h)$ instead, which is defined as

$$C(h) = E [Z(x) \cdot Z(x + h)] - m^2, \quad (3.3)$$

where $E[\xi]$ is the mathematical expectation operator¹, and m is the mean. A variogram function can be deduced from a covariance function by means of the formula

$$\gamma(h) = C(0) - C(h). \quad (3.4)$$

However, the reverse is only true when the variogram is bounded within the framework fixed by second order stationarity.

The variogram model obtained is used in the computation of the weights by solution of the following ordinary kriging system of linear equations:

$$\begin{cases} \sum_{\beta=1}^n w_\beta \gamma(x_\alpha - x_\beta) + \mu = \gamma(x_\alpha - x_0) \\ \sum_{\beta=1}^n w_\beta = 1 \end{cases} \quad \text{for } \alpha = 1, \dots, n. \quad (3.5)$$

The functions $\gamma(x_\alpha - x_\beta)$ and $\gamma(x_\alpha - x_0)$ respectively represent the model variogram for pairs of sampled points and the variogram between sampled points and the point to be estimated. The ordinary kriging system of linear equations has

¹This is a linear operator defined as $E[\xi] = \sum_{i=1}^n p_i \xi_i$ in its discrete formulation, where p_i is the probability associated with the i th observation of ξ .

the restriction that the weights must sum up to 1, which is achieved by the introduction of the Lagrange parameter μ in the derivation of the kriging equations. In this derivation the objective is to minimize the error variance and ensuring that, on average, the estimating error is zero. Therefore, kriging is usually referred as the best linear unbiased estimator. An important note to keep in mind is that when data follows a normal distribution, the distribution of the kriging estimates are conform with that of the original data values (this is actually the most favorable situation). However, not always we are in the presence of normal distributions, and when this happens, the distribution of the estimates may deviate considerably from that of the original data. As a final result, this is very poor but it is sometimes possible to correct by transforming the original data in a normal distribution before kriging is performed [13].

3.1. Ordinary lognormal kriging

Ordinary kriging corresponds to the simplest case of kriging estimation, and it has been shown that normally distributed data is the most favorable situation for the use of kriging as an estimation technique. However, it has been verified for some time that most distributions in geochemistry (especially for minor elements which are the most important to mining) show log-normal distributions (the work of de Wijs [19] is just an example), and ordinary kriging may fail to give estimates following the same distribution as the original data.

Let $Z(x)$ be a stationary random function with a multivariate log-normal distribution, an expectation m , a covariance function $C(h)$ and a variance $\sigma^2 = C(0)$. Then,

$$Y(x_\alpha) = \log Z(x_\alpha) \text{ for } \alpha = 1, \dots, n \quad (3.6)$$

yields a new random function $Y(x)$ with a multivariate normal distribution with expectation m' , covariance function $C'(h)$ and variance $\sigma'^2 = C'(0)$. Therefore, the variable $Y(x_\alpha)$ may be linearly estimated at a given location (x_0) using the equation

$$y^*(x_0) = m_y + \sum_{\alpha=1}^n w_\alpha (y(x_\alpha) - m_y)^2, \quad (3.7)$$

where m_y is the mean of $Y(x)$ and w_α are the kriging weights computed with the ordinary kriging system of equations (3.5) [13]. An estimation of $Z(x_\alpha)$ is obtained by the back transformation of the estimated values of $Y(x_\alpha)$, however

not by the simple inversion of equation (3.6). Instead

$$z^*(x_0) = X_{K_0} \exp \left(y^*(x_0) + \frac{\sigma_{K_0}^2}{2} \right), \quad (3.8)$$

where $\sigma_{K_0}^2$ is the kriging variance of the estimation of $Y(x_\alpha)$ and X_{K_0} is a correction factor given by the ratio of the mean of the original data to the mean of the estimates [13]. The correction factor may then be tested by cross-validation, *i.e.*, given a set of n samples, for each point where a sample exists a value is estimated using all the $n - 1$ samples (excluding the one at that location). The mean difference between the estimated and true values, done for all data set, should be close to zero, as required by the derivation of the kriging equations. The expression (3.8) arises due to lack of robustness of the exponential term with regard to the multivariate log-normal hypothesis [13].

3.2. Factorial kriging

A regionalized phenomenon can be thought as being the contribution of several independent subphenomena acting at different characteristic scales. A linear model may be set up as a sum of uncorrelated random functions, each one with its own variogram or covariance function.

This model can be directly transferred to the problem of geochemical anomaly definition. We may conceive an area where a series of mineralized bodies occur, releasing to the soil a set of indicative chemical elements. We know that orebodies do not have regular and constant grades. Instead, there are different parts of an orebody which are richer than others (sometimes significantly richer). We could also think in a particular rock type (lets call it rock A) where the concentration of a chemical element is, on average, higher than in the rest of the rocks, which dominate in the area. It might also happen that an enrichment of that element has occurred within rock A . Therefore, all these variations in the rocks may also be reflected in the soils covering the area. In this example, lets cover all the area with a sampling grid where a soil sample is taken at each node, and analyze it for the element of interest; what will be the variation of the concentration of the element in the soil as a function of its position? We may find average concentrations of the element as a consequence of the contribution of the majority of the rocks present in the area, and this concentration can be viewed as the regional background concentration of the element in the area. However, as one moves over the rock A , the average concentrations in the samples are higher

than in the previous case and evidence what we may call as a regional anomaly, since the main contribution is from a particular rock type. For samples over the enriched zones, these average concentrations may rise even more and we are faced with an anomaly at a local scale, which may be just one sample, depending on the size of the enriched zone and on the sample spacing. The underlying physical phenomenon for the concentration of the element in each of these cases is different, because the way rocks are formed depend on their identity, and the enriched zone may form by totally independent processes from the ones that form the host rock (the enrichment does not even need to be formed at the same time as the rock, which is the most common case).

Each of these concentrations have characteristic scales, *i.e.*, the regional background concentrations are spread all over the area, and samples show long-range correlations. The local anomalous concentrations are restricted to the neighborhood of rock *A* and only a limited number of samples show those values, therefore having a short-range correlation. Local anomalous concentrations may be restricted to isolated samples, and if great variations occur at a length scale lesser than sample spacing, then we have the expression of what is called a *nugget effect*.

The model variogram for this set of measurements may reveal all these structures. The experimental variogram can be modeled as a sum of elementary variogram functions, each one with different sills revealing each spatial characteristics of the data at a given scale. A *nested variogram model* is then formed, by adding the n elementary variograms each one with coefficients b^u as

$$\gamma(h) = \sum_{u=1}^n \gamma^u(h) = \sum_{u=1}^n b^u g^u(h), \quad (3.9)$$

where $g^u(h)$ represent the normalized variograms.

A second-order stationary random function, $Z(x)$, can be built by adding the uncorrelated stationary random functions $Z^u(x)$ to a constant m , which is the expectation of $Z(x)$:

$$Z(x) = \sum_{u=1}^n Z^u(x) + m. \quad (3.10)$$

The objective is to map each of these components of the random function $Z(x)$, and is the basis of *factorial kriging*.

Factorial kriging was first developed by Matheron [15] with the objective of decomposing the regionalized variable into components which can be mapped separately. The problem may be treated as univariate [17] or multivariate, when more

than one variable is considered relevant to the problem [16, 12]. The experimental variogram is the basic tool to reveal such components which, as can easily be deduced from the example given above, it is the most frequent case to occur in geochemical analysis. Only the univariate case will be very shortly presented.

The components of regionalization models can be extracted or, in a complementary way, filtered using kriging. For $Z(x)$ defined by equation (3.10), we may wish to estimate a particular second-order stationary component $Z^u(x)$, which we do with the following linear combination:

$$Z^{u*}(x_0) = \sum_{\alpha=1}^n w_{\alpha}^u Z(x_{\alpha}). \quad (3.11)$$

Unbiasedness is achieved on the basis of zero sum weights, and the kriging system for the component $Z^u(x_0)$ is [18]

$$\left\{ \begin{array}{l} \sum_{\beta=1}^n w_{\beta}^u \gamma(x_{\alpha} - x_{\beta}) + \mu^u = \gamma^u(x_{\alpha} - x_0) \\ \sum_{\beta=1}^n w_{\beta}^u = 0 \end{array} \right. \quad \text{for } \alpha = 1, \dots, n. \quad (3.12)$$

Note that in the right hand side of equation (3.12) only the variogram function associated with the structure to be mapped appears.

4. MULTIFRACTAL SETS AND SELF-SIMILAR MEASURES

The idea of multifractal modeling of geochemical data sets have been applied in several studies [2, 3, 4]. As pointed out by Evertsz and Mandelbrot [6], multifractals is the name by which the theory of self-similar measures is usually known. These same authors give a simple image of a multifractal using ground water as an example. Consider a region in a map (domain) and define μ as 'the amount of ground water in the region'. To each subset of the map, the measure attributes a quantity $\mu(S)$, which is the amount of ground water below S , down to some prescribed level. If the domain is sub-divided into two equally sized subsets, S_1 and S_2 , the most probable thing to happen is that $\mu(S_1) \neq \mu(S_2)$. If these subsets are further divided into two equally sized pieces, S_{11} and S_{12} , and S_{21} and S_{22} , their ground water contents still differ from each other, and so on. It is not very hard to imagine this same picture referring to the distribution of some chemical element at the surface of the Earth.

In the simple and straightforward method of fractal measures, it is not enough to consider a collection of boxes of size ϵ , covering S , in the example above, and getting a relation of the type $N(\epsilon) \sim \epsilon^{-D}$. There is a fundamental knowledge, which is the measure, that is lacking in that description. Self-similar measures have a quantity defined by

$$\alpha = \frac{\log \mu(\text{box})}{\log(\epsilon)}, \quad (4.1)$$

called the *coarse Hölder exponent*, where the logarithm of the measure of the box is divided by the logarithm of the size of the box. For a large class of self-similar measures, α is restricted to the interval $[\alpha_{\min}, \alpha_{\max}]$, where $0 < \alpha_{\min} < \alpha_{\max} < \infty$. For each value α , the number of boxes having a coarse Hölder exponent equal to α , $N_\epsilon(\alpha)$, is evaluated. If a box of size ϵ is selected at random among boxes whose total number is proportional to ϵ^{-E} , the probability of hitting the value α of the

coarse Hölder exponent is

$$p_\epsilon(\alpha) = \frac{N_\epsilon(\alpha)}{\epsilon^{-E}}. \quad (4.2)$$

It is then necessary to consider either of the functions [6]

$$f_\epsilon(\alpha) = -\frac{\log N_\epsilon(\alpha)}{\log \epsilon}, \quad (4.3)$$

or

$$C_\epsilon(\alpha) = -\frac{\log p_\epsilon(\alpha)}{\log \epsilon}. \quad (4.4)$$

As $\epsilon \rightarrow 0$, both $f_\epsilon(\alpha)$ and $C_\epsilon(\alpha)$ tend to well defined limits $f(\alpha)$ and $C(\alpha)$. The function $f(\alpha)$ is called the multifractal spectrum, and when exists

$$C(\alpha) = f(\alpha) - E. \quad (4.5)$$

The definition of $f(\alpha)$ means that, for each α , the number of boxes increases for decreasing ϵ and $N_\epsilon(\alpha) \sim \epsilon^{-f(\alpha)}$. The exponent $f(\alpha)$ is a continuous function of α , and in the simplest cases it has the shape of the mathematical symbol \cap . As $\epsilon \rightarrow 0$, there is an increasing multitude (up to infinity) of subsets, each characterized by its own α , and a fractal dimension $f(\alpha)$ - therefore the name of multifractals. The function $f(\alpha)$ has one, and only one, maximum which is coincident with the fractal dimension determined by the box counting method [10].

4.1. Estimating $f(\alpha)$ experimentally from data

Having a set of measurements, we may be interested to know how we could determine if this set of measures is multifractal or not. The way we may answer this question is, once more, given by Evertsz and Mandelbrot [6] which present some methods of estimating the $f(\alpha)$ function experimentally from data. The method transcribed bellow is the *Method of Moments*, which has also been applied by [4] and [1] to model geochemical data and fractures respectively, and will be discussed later. The method is based on a quantity called the *partition function*. Suppose $\mu(S)$ represents a measure of a set S in \mathfrak{R}^n . The set may be partitioned into $N(\epsilon)$ cells of equal size ϵ . The value $\mu_i(\epsilon)$ stands for the measure on S for the i th cell of size ϵ . The partition function is then defined as

$$\chi_q(\epsilon) = \sum_{i=1}^{N(\epsilon)} \mu_i^q(\epsilon), \quad q \in \mathfrak{R}. \quad (4.6)$$

The measure μ_i of the boxes may be rewritten as $\mu_i = \epsilon^{\alpha_i}$, yielding $\chi_q = \sum_{i=1}^{N(\epsilon)} (\epsilon^{\alpha_i})^q$. We may also denote by $N_\epsilon(\alpha)d\alpha$ the number of boxes out of the total $N(\epsilon)$ for which the coarse Hölder exponent satisfies $\alpha < \alpha_i < \alpha + d\alpha$, and assume that the constants α_{\min} and α_{\max} exist and satisfy $0 < \alpha_{\min} < \alpha < \alpha_{\max} < \infty$ and that $N_\epsilon(\alpha)$ is continuous. The contribution of the subset of boxes with α_i between α and $\alpha + d\alpha$ to $\chi_q(\epsilon)$ is $N_\epsilon(\alpha)(\epsilon^\alpha)^q d\alpha$. In order to add the contribution of subsets whose coarse Hölder exponent is between α and $\alpha + d\alpha$, the equation (4.6) is integrated over $d\alpha$, yielding

$$\chi_q(\epsilon) = \int N_\epsilon(\alpha)(\epsilon^\alpha)^q d\alpha. \quad (4.7)$$

We have seen already that we may have $N_\epsilon(\alpha) \sim \epsilon^{-f(\alpha)}$, thus

$$\chi_q(\epsilon) = \int \epsilon^{\alpha q - f(\alpha)} d\alpha. \quad (4.8)$$

In the limit $\epsilon \rightarrow 0$, the dominant contribution to the integral comes from α values close to the value that minimizes the exponent $q\alpha - f(\alpha)$. If $f(\alpha)$ is differentiable and replacing α by $\alpha(q)$, defined by the extremal condition, we obtain [10, 6]

$$\left. \frac{\partial}{\partial \alpha} \{q\alpha - f(\alpha)\} \right|_{\alpha=\alpha(q)} = 0, \quad (4.9)$$

and

$$\left. \frac{\partial^2}{\partial \alpha^2} \{q\alpha - f(\alpha)\} \right|_{\alpha=\alpha(q)} > 0. \quad (4.10)$$

Therefore, we find that

$$\left. \frac{\partial f(\alpha)}{\partial \alpha} \right|_{\alpha=\alpha(q)} = q \quad (4.11)$$

satisfies such condition for the value of $\alpha = \alpha(q)$ and this extremum is a minimum if

$$\left. \frac{\partial^2 f(\alpha)}{\partial \alpha^2} \right|_{\alpha=\alpha(q)} < 0. \quad (4.12)$$

Therefore, the function $f(\alpha)$ should be cap convex as it was already referred in the introductory part, and for the $\alpha = \alpha(q)$ where the minimum is attained, the slope of $f(\alpha)$ is q .

Therefore, if the measure $\mu_i(\epsilon)$ satisfies the multifractal model, we may find that the partition function (4.6) has a power-law relation with the cell size ϵ for any order q , where $-\infty \leq q \leq \infty$, which means

$$\chi_q(\epsilon) \sim \epsilon^{\tau(q)}. \quad (4.13)$$

The function $\tau(q)$, is called the mass exponent of order q , and is given by (see equation 4.8)

$$\tau(q) = q\alpha(q) - f(\alpha(q)). \quad (4.14)$$

The singularity exponent $\alpha(q)$ may then be obtained from the expression

$$\frac{\partial \tau(q)}{\partial q} = \alpha(q), \quad (4.15)$$

and the multifractal spectrum $f(\alpha)$ can be obtained from $\tau(q)$ using equation (4.14), rearranging to

$$f(\alpha(q)) = q\alpha(q) - \tau(q). \quad (4.16)$$

The equation (4.16) is called the *Legendre transform* of $\tau(q)$.

In the general case, there is a lack of theoretical knowledge of the physical phenomenon we are studying implying that the computation of the $f(\alpha)$ function must be carried out numerically instead of analytically. To compute $f(\alpha)$ using the partition function requires to follow a series of steps which will be described next [6].

- Cover all the domain with a set of boxes $\{B_i(\epsilon)\}_{i=1}^{N(\epsilon)}$ of size ϵ and determine the corresponding box measure $\mu_i = \mu[B_i(\epsilon)]$;
- Compute the partition function in equation (4.6) for various values of ϵ ;
- If the plots of $\log \chi_q(\epsilon)$ versus $\log \epsilon$ follow straight lines, $\tau(q)$ is the slope corresponding to a given exponent q ;
- Compute the value of $\alpha(q)$ from equation (4.15) using a finite difference method;
- Form $f(\alpha)$ from the Legendre transform of $\tau(q)$ (equation 4.16).

It is very important to stress that Evertsz and Mandelbrot [6] make a severe warning about the measure performed. While performing the third step above, all points must be in a straight line, and if, instead, a fitted straight line is obtained by a least square method, the result may be statistically rigorous but may turn out to be physically meaningless.

The method of the moments suggest that a measure is multifractal if, and only if, the function $\tau(q)$ exist for all $q \in \mathfrak{R}$. However, measures that fullfil this condition should be termed *restricted multifractals*, since some measures, although multifractal, fail to comply to this criterion.

4.2. Applications of multifractal modeling

As already mentioned, some work has been done by applying the above methodology to geochemistry and also fracture networks, proposing a bridge between multifractal modeling and geostatistical analysis [4]. This study used the famous de Wijs [19] zinc assay values, which is a work about the distribution of ore elements advancing with some ideas of dealing with the problem similar to the ones of present-day self-similar measures. The zinc assay values is a one dimensional measuring problem, which is not very difficult to handle. As to the problem of fracture network modeling [1], we face a two dimensional measuring problem which is similar to the analysis of soil geochemistry. In this work, the authors had to account with the subdivision of the area into equally sized cells with different dimensions ϵ , and with the fact that, since the analysis is performed over a mapped region, the outcropping rocks do not occupy the entire cell. As a matter of fact, this situation is the commonest one. Therefore, in the use of the partition function equation (4.6), they had to introduce a parameter to make the measure unbiased. This parameter is a weight defined as $w_i = s_i/a$ for $i = 1, \dots, n$, where s_i is the area of the exposed bedrock per cell, and a is the cell area, therefore equation (4.6) becomes [1]

$$\chi_q(\epsilon) = \sum_{i=1}^{N(\epsilon)} w_i \left[\frac{\mu_i(\epsilon)}{w_i} \right]^q, \quad q \in \mathfrak{R}. \quad (4.17)$$

This equation reduces to (4.6) when $q = 1$, and implies that the exposed part of the cell is representative for the entire cell.

The problem, when addressed to soil geochemistry, is very similar but some details must be emphasized. When we deal with regularly spaced data, the problem is very much simplified, but only to a limited extent. In this case, we may

choose a grid cell size such that a single sample point falls in each cell (actually, the smallest possible cell to use), and the measure to perform is equal to the point value. However, when we consider larger grid cells (which may also be considered similar to the case of irregularly spaced data), several point values may fall within each cell, and we ask: what is the measure for this cell? The simple question of averaging the values is not as straightforward as it seems, although Cheng and Agterberg [4] have applied it to the de Wijs example. Geostatistics has developed as a branch of applied mathematics precisely to deal with distributions of variables in space whose value is not independent of their position, therefore, it seems rather dull just to forget this and deal with data in a conventional statistical way. The problem of measure here is also a problem of estimation, and geostatistics can not be regarded separately from this problem. Therefore, the problem of the measure should be addressed by solving the set of kriging equations as when block estimates are made (*e.g.* [11]). Following the work presented in [7], the test of the multifractal model was made to this data set, and results always fail to prove it as multifractal in nature (Gonçalves, unpublished data). Several reasons may be put forward to explain such failure: difficulties of grid subdivision due to very irregular shape of the covered area; a large number of values (more than 50%) bellow the detection limit of the analytical method; poor quality of the data in a general way, not only due to the previous reason, but also because two sampling campaigns were performed in different conditions. The problem of handling values bellow detection limit is a very problematic one, and to the author's knowledge, nobody ever referred such problems and how to handling them. Such a measure only tells us that the concentration is bellow a given value, and cannot either be estimated by kriging nor even ignored. Therefore, without having a reliable method of handling this sort of data, the applicability of the methods discussed until now may be very limited. However, it is quite striking to observe that the data of [7] as well as of [8] can be very well fitted by the models of equations (2.3) to (2.5). In the first case, it was impossible to prove the multifractal model, and in the second case this was never attempted. Still, the results obtained correlate very well with the geological knowledge of the studied areas, and the calculated geochemical threshold values are very close to the mean value content exhibited by the host rocks responsible for the anomalies. We may ask next if between equations (2.3) to (2.5) and the multifractal model is there any relation at all. It seems that for the tested data set [7], the assumption of the multifractal model is perfectly irrelevant. However, regarding the difficulties in data handling and its questionable quality, this statement should be taken more carefully. In the test of

the multifractal hypothesis to the data set of [7], the measures in each box were obtained by averaging the enclosed values, but we have put severe reserves to this simple and straightforward method. This measure must be obtained by means of block kriging estimation.

5. CONCLUSIONS

After the presentation of the above methods and their applicability, we should make a synthesis, and propose possible directions of future research of the problem. Both, the geostatistical and multifractal approaches have given results which prove that the methods are efficient, at least to a certain degree. However, the computational requirements for each is very different, and the multifractal method is far more simple in some circumstances. At least, even for data sets that, apparently, do not comply to the multifractal model, the multifractal approach still gives reliable predictions about the definition of anomalous areas. However, the information must always be integrated with data from other sources. At this stage of the research it is not proven that the methodology is universal, therefore the comparison of results is still fundamental. At least the approach to two dimensional spatial data, the performance of self-similar measurements still requires the use of kriging, by means of the block kriging equations since we are measuring boxes (or blocks).

The application of factorial kriging is self-consistent with all the geostatistical framework, and the efficiency of the results is well proven. Information from other sources is also needed, since the results may not be readily interpreted. This methodology does not give a quantitative value for the anomalous threshold in an area, instead produces a map of the different components of the random function which, in turn, may or may not be spatially related to orebodies or other types of geological structures responsible for the anomalies.

A comparative study of both methodologies should be made in order to quantify the fitness of the results produced by these methods. If both methods are in well agreement, a possible line of research could be the integration of the methods in a robust framework, aimed at the identification of spatial geochemical anomalies.

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