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Multifractals and geostatistics

F.P. Agterberg *

Geological Survey of Canada, 601 Booth Street, Ottawa, Ont., Canada, K1A 0E8

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ABSTRACT

In several recent studies, 2-dimensional applications of local singularity analysis including regional studies based on stream sediment data show local minima that are spatially correlated with known mineral deposits. These minimal singularities, which may provide targets for further mineral exploration, generally are smoothed out when traditional geostatistical contouring methods are used. Multifractal analysis based on the assumption of self-similarity predicts strong local continuity of element concentration values that cannot be readily determined by variogram or correlogram analysis. This paper is concerned with multifractal and geostatistical modeling of the largest and smallest geochemical element concentration values in rocks and orebodies. These extreme values correspond to local singularities with near-zero fractal dimensions that occur close to the minimum and maximum singularity in the multifractal spectrum. The latter cannot be determined by means of the method of moments because of small-sample size problems arising when the largest and smallest concentration values are raised to very large powers q. It is shown by means of a computer simulation experiment and application to copper determinations from along the 7-km deep KTB borehole in southeastern Germany, that local singularity analysis can be used to determine all singularities including the extreme values. The singularities estimated by this method are linearly related to logarithmically transformed element concentration values. This simple relation also can used to measure the small-scale nugget effect, which may be related to measurement error and microscopic randomness associated with ore grain boundaries.

1. Introduction

During the past 40 years, the fractal geometry of many natural features in Nature has become widely recognized (see e.g. Barnsley, 1988; Carranza, 2008; Mandelbrot, 1983; Raines, 2008; Turcotte, 1997). Fractals in geology either represent the end products of numerous, more or less independent processes (e.g. coastlines and topography), or they result from nonlinear processes, many of which took place long ago within the Earth's crust. Although a great variety of fractals can be generated by relatively simple algorithms, theory needed to explain fractals of the second kind generally is not so simple, because previously neglected nonlinear terms have to be inserted into existing linear, deterministic equations. Several types of patterns are best modeled as multifractals, which are spatially intertwined fractals (Stanley and Meakin, 1988). Most progress in multifractal theory development has been made in geophysics to study nonlinear processes including cloud formation and rainfall (Schertzer and Lovejoy, 1991). Lovejoy and Schertzer (2007), Lovejoy et al. (2008), Cheng (2008), Ford and Blenkinsop (2009), Agterberg (2012) and Cheng (2012) show that scaling and multifractal fields also exist within solid Earth.

In this paper special attention will be paid to sampling problems which arise because chemical concentration values for small rock samples must be extrapolated over much larger rock masses in order to describe the multifractal fields. Such extrapolations remain subject to uncertainty. Much of classical theory of mathematical statistics is based of random variables for measurements that are stochastically independent. In general, chemical determinations for rock samples are subject to spatial dependence and use can be made of geostatistical theory originally developed by Matheron (1962), whose geometrical approach is also explained in various geostatistical textbooks including David, 1977, Journel and Huijbregts (1978) and Cressie (2001). Matheron (1962) initially based his geostatistical theory on the principle of "similitude" underlying the model of de Wijs (1951). Later, Mandelbrot (1983) recognized that it can be said that de Wijs (1951) developed the first multifractal also known as the p-model (Schertzer et al., 1997) or binomial/p model (Lovejoy and Schertzer, 2007). Krige (1978) demonstrated that the model of de Wijs could be applied to hundreds of thousands of gold assays from Witwatersrand goldfields, at scales ranging from local to regional (see also Mandelbrot, 1995).

The model of de Wijs is based on the simple assumption that when a block of rock with an element concentration value X is divided into two halves, the element concentration values of the two halves are $(1+d)\cdot X$ and $(1-d)\cdot X$ regardless of the size of the block. The coefficient d is the index of dispersion. The ratio $(1+d)/(1-d)$ can be written as $\eta > 1$. The process of starting with one block that is divided into halves, dividing

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* Geological survey of Canada, 601 Booth Street, Ottawa, Canada, K1A 0E8. Tel.: +1 613 9962374.

E-mail addresses: Frits.Agterberg@NRCan-RNCan.gc.ca, agterber@nrcan.gc.ca.

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the halves into quarters and continuing the process of dividing the smaller blocks into halves represents a multiplicative cascade. This model resulting in self-similarity or scale independence can be readily generalized in two ways: (1) in practical applications there generally is a lower limit to the size of blocks with the same index of dispersion as larger blocks. Below this limit, d usually decreases rapidly to zero; this limitation is accommodated in the 3-parameter model of de Wijs (Agterberg, 2007a) that has an effective maximum number of subdivisions beyond which the model of constant index of dispersion does not apply; (2) the idea of cutting any block into halves with constant value of d is not realistic on a local scale (e.g. d does not stay exactly the same when halves become quarters). However, this problem is eliminated in the random cut model for which the coefficient d is replaced by a random variable D with variance independent of block size (Agterberg, 2007a). The end products of constant dispersion and random cut cascades are similar.

To illustrate application of his model, De Wijs (1951) used a series of 118 zinc concentration values from channel samples taken at a regular 2-m interval along a horizontal drift in the Pulacayo zinc deposit, Bolivia (Fig. 2, see later). This series was used extensively for later study in geostatistics and multifractal modeling, not only by Matheron (1962), but by several other authors including Agterberg (1967,1994), Cheng and Agterberg (1996), Chen et al. (2007), Lovejoy and Schertzer (2007) and Agterberg (2012). In this paper, multifractal modeling will be applied to an artificial series in a computer simulation experiment and to a series of 1796 copper concentration values from along a section of the 7-km deep KTB borehole drilled in the Bohemian Massif in southeast Germany.

The model of de Wijs results in a logbinomial frequency distribution of element concentration values (X) with logarithmic variance:

$$\sigma^2(\ln X) = n\cdot(\ln\eta)^2/4. \tag{1}$$

According to the De Moivre–Laplace theorem (Bickel and Dockum, 2001, p. 470), the frequency distribution of ln X converges to normal form when n increases. Frequency density values in the upper tail of the logbinomial are less than those of the lognormal. The logbinomial would become lognormal when n representing the number of subdivisions of blocks is increased indefinitely. Paradoxically, its variance then also would become infinitely large. In practical applications, it is often seen that the upper tail of a frequency density function of element concentration values is not thinner but thicker and extending further than a lognormal tail. Several cascade models (e.g. Veneziano and Langousis, 2005) result in frequency distributions that resemble the lognormal but have Pareto tails. Already in the 1980s, Schertzer and Lovejoy (1985) had pointed out that the binomial/p model can be regarded as a “micro-canonical” version of their α-model in which the strict condition of local preservation of mass is replaced by a more general condition of preservation of mass within wider neighborhoods (preservation of ensemble averages). Cascades of this type can result in lognormals with Pareto tails. In the 3-parameter Lovejoy–Schertzer α-model, α is not the singularity but represents the Lévy index that, together with “codimension” C_1 and “deviation from conservation” H, characterizes the multifractal field. Examples of applicability of these approaches to geological processes that took place in the Earth's crust have been given by Lovejoy and Schertzer (2007).

Another possible explanation of thicker, longer tails of frequency distributions of geochemical data is provided by the following variant of the model of de Wijs in which the coefficient of dispersion (d) increases with element concentration value X during the multiplicative cascade process, or

$$d = d_0 \exp(-p\cdot X) \tag{2}$$

where d_0 represents initial dispersion index, at the beginning of the multiplicative cascade, and p is a constant. This accelerated dispersion model produces thicker and longer than lognormal frequency distribution tails (Agterberg, 2007b). Additionally, it yields more very small values thus producing a secondary peak near the origin of the frequency density function. Cheng (2008, 2012) has proposed that very large element concentration values, which correspond to relatively low singularities, are spatially correlated to mappable properties of rocks. It is possible that the latter are related to relatively large value of the constant (p) in Eq. (2) that significantly affects the largest (and smallest) values only.

Matheron (1962) generalized the original model of de Wijs by introducing the concept of “absolute dispersion” here written as $A = (\ln \eta)^2/\ln 16$. This approach is equivalent to what is now better known as scale invariance. It leads to the more general equation

$$\sigma^2(\ln X) = A\cdot \ln\{V/v\} \tag{3}$$

where σ^2 (ln X) represents logarithmic variance of element concentration values X in smaller blocks with volume v contained within a larger block of rock with volume V.

Fig. 1 is a classical example of the relationship between logarithmic variance and block size for Witwatersrand gold values as derived by Krige (1966). The gold occurs in relatively thin sedimentary layers called “reefs”. Average gold concentration value is multiplied by length of sample cut across reef and unit of gold assay values is expressed as inch-pennyweight in Fig. 1 (1 inch-pennyweight = 3.95 cm-g). Three straight-line relationships for smaller blocks within larger blocks are indicated. However, there are two departures from the simple model of Eq. (3). The first of these departures is that a small constant term (+20 inch-pennyweights) was added to all gold values. This reflects the fact that, in general, the 3-parameter lognormal model provides a better fit than the 2-parameter lognormal (Krige, 1966). As discussed in more detail in Agterberg (1974, pp. 216–217), this departure corresponds to a narrow, secondary, peak near the origin of the normal Gaussian frequency density curve for logarithmically transformed gold concentration values (Agterberg, 1974, Fig. 32). The accelerated dispersion model of Eq. (2) would explain this type of secondary peak. The second departure consists of constant terms that are contained in the observed logarithmic variances plotted in Fig. 1. These additive terms are related to differences in shapes of the blocks with volumes v and V as will be explained in more detail in the next section.

Geostatistical studies commonly are based on a semivariogram fitted to element concentration values from larger neighborhoods. Generally, these models show a “nugget effect” at the origin, a “range” of significant spatial autocorrelation with a “sill” that corresponds to regional mean concentration value. It is well known that the “nugget effect” generally is much larger than chemical determination errors and microscopic randomness associated with ore grain boundaries. This second source of randomness arises because, at the microscopic level, chemical elements generally are confined to crystals with boundaries that introduce randomness at very small scales. In general, the preceding two sources of local randomness have effects that rapidly decline with distance. Local clustering of ore crystals at scales less than the sampling interval used for sampling rocks or orebodies is probably widespread. Multifractal semivariograms can account for local continuity due to clustering (Agterberg, 2012). Similar local continuity effects exist in other types of data; e.g., data resulting from stream sediment geochemical surveys.

Most geological maps display bedrock as a mosaic of distinct rock units of different composition and age. Small rock samples are taken and subjected to chemical analysis. Normally, the resulting chemical element concentration values are used to help with rock identification and to describe the physico-chemical processes that led to the patterns of rock units on the geological map and its three-dimensional extensions into depth. Although orebodies and hydrocarbon deposits generally occupy relatively small volumes within the Earth's crust, they are targets of intense exploration including chemical determinations both