Computers & Geosciences 105 (2017) 139–147

Contents lists available at ScienceDirect

Computers & Geosciences

journal homepage: www.elsevier.com/locate/cageo

Research paper

A new method for geochemical anomaly separation based on the distribution patterns of singularity indices

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ARTICLE INFO

Key words:
Singularity analysis
Quantile-quantile plot
Geochemical anomaly separation
MaxEnt model
Chromitite exploration
Western Junggar region

ABSTRACT

Singularity analysis is one of the most important models in the fractal/multifractal family that has been demonstrated as an efficient tool for identifying hybrid distribution patterns of geochemical data, such as normal and multifractal distributions. However, the question of how to appropriately separate these patterns using reasonable thresholds has not been well answered. In the present study, a new method termed singularity-quantile (S-Q) analysis was proposed to separate multiple geochemical anomaly populations based on integrating singularity analysis and quantile-quantile plot (QQ-plot) analysis. The new method provides excellent abilities for characterizing frequency distribution patterns of singularity indices by plotting singularity index quantiles vs. standard normal quantiles. From a perspective of geochemical element enrichment processes, distribution patterns of singularity indices can be evidently separated into three groups by means of the new method, corresponding to element enrichment, element generality and element depletion, respectively. A case study for chromitite exploration based on geochemical data in the western Junggar region (China), was employed to examine the potential application of the new method. The results revealed that the proposed method was very sensitive to the changes of singularity indices with three segments when it was applied to characterize geochemical element enrichment processes. And hence, the S-Q method can be considered as an efficient and powerful tool for separating hybrid geochemical anomalies on the basis of statistical and inherent fractal/multifractal properties.

1. Introduction

How to efficiently distinguish geochemical anomalies from background, aiming for mineral resource assessment, is still one of the most important concerns faced by exploration geochemical data processing. The challenge for geochemical anomaly identification is to determine reasonable thresholds for separating anomalies from background. In the past several decades, various methods have been applied for geochemical anomaly identification and threshold separation, mainly including frequency-based univariate statistical methods (Sinclair, 1974; Stanley and Sinclair, 1987; Carranza, 2010, 2011), multivariate statistical methods (Reimann et al., 2002; Yousefi et al., 2012, 2013, 2014; Liu et al., 2014a; Geranian et al., 2015; Gonbadi et al., 2015; Nazarpour et al., 2016), and power-law based fractal/multifractal models (Afzal et al., 2013; Cheng et al., 1996, 2000; Cheng, 2007, 2012; Goncalves et al., 2001; Zhao et al., 2012; Liu et al., 2013, 2014b; Xie and Bao, 2004; Arias et al., 2012; Zuo et al., 2013; Agterberg, 2014; Luz et al., 2014; Khalajmasoumi et al., 2016; Parsa et al., 2016). Traditional univariate and multivariate statistical methods are suitable for processing dataset with normal or lognormal distributions, whether or not these methods are applied in frequency domain or/and space domain (Ahrens, 1954; Miller and Goldberg, 1955; Xie et al., 2007). Therefore, geochemical anomalies with extreme values might be not detected from background by these traditional statistic methods, especially when weak anomalies are hidden in complex geological settings or the difference between anomaly and background is feeble (Cheng, 2007).

In the past two decades, many power-law based fractal/multifractal models have been developed for mineral exploration, such as the singularity analysis (Cheng, 2007, 2015), concentration–area fractal model (C-A; Cheng et al., 1994), spectrum–area model (S-A; Cheng et al., 2000), concentration–distance model (C-D; Li et al., 2003),

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http://dx.doi.org/10.1016/j.cageo.2017.05.008
Received 11 January 2017; Received in revised form 17 April 2017; Accepted 17 May 2017
Available online 18 May 2017

spectrum–volume model (S-V; Afzal et al., 2012), concentration–volume model (C-V; Afzal et al., 2011), ore deposit fractal clustering (Carlson, 1991; Blenkinsop, 1994; Gumiel et al., 2010); and wavelet-based multiscale decomposition model (WMD; Chen and Cheng, 2016), among which singularity analysis is one of the most important models in the fractal/multifractal family that has been widely applied for geochemical anomaly identification (Chen et al., 2007; Xiao et al., 2012, 2016; Cheng, 2007, 2012; Liu et al., 2013, 2014b; Wang et al., 2012, 2015; Zuo et al., 2009; Agterberg, 2012a; Zuo and Wang, 2016). From a geochemical point of view, singularity analysis accentuates crucial changes in geochemical element concentration and changes in measureable physical properties of geochemical data.

Many, if not most, ore deposits are the products of multiple ore-forming processes in complex geological settings, accompanying different geological processes, such as magma hydrothermalism, deposition process, tectonic cycles, metamorphism, mineralization, that overlapped each other spatially and temporally (Robb, 2005). This phenomenon of metal mineralization can be considered as a type of singular geophysical and geochemical processes occurred in relatively narrow space and/or time intervals, accompanied by anomalous mass accumulation and/or energy release. As described by Cheng (2007), singularity is a fundamental property of complex ore-forming processes caused by intensive element enrichment, which can be measured by fractal/multifractal distributions. Normal/lognormal and fractal/multifractal or Pareto distributions are commonly applied in the investigation of geochemical data, since these distribution patterns can describe good approximations of geochemical concentration values of various sampling media (e.g., rocks, soils, stream sediments, etc; Cheng, 2008; Agterberg, 2007, 2017). However, geochemical anomalies and their explanation are not always obvious on visual inspection or purpose exploratory investigation. In the present study, the proposed S-Q method based on singularity analysis and QQ-plot analysis was used to separate hybrid distribution patterns of singularity indices and to express the results graphically. The method considers the inherent fractal/ multifractal properties, and its potential application was demonstrated by a case study for chromitite exploration in the western Junggar region, China.

2. Methods

2.1. Singularity analysis

The end products of mineralization processes can be modeled as fractals or multifractals, because of the regularity of enrichment and dispersion of geochemical element concentrations (Cheng, 2007, 2008). For 2-dimensional exploration geochemical data from surface samples, singularity analysis uses so called singularity index (α) to characterize geochemical complexity that is related to metal mineralization within a multifractal context (Cheng, 2007, 2012; Cheng and Agterberg, 2009; Agterberg, 2012b). Suppose that $\mu(A)$ is the total amount of element concentration within an area A, and $\rho(A)$ is the density of element concentration within an area A. From a multifractal point of view, the $\mu(A)$ and $\rho(A)$ follow power-law relationships expressed by:

$$\mu(A) \propto A^{\alpha/2} \tag{1}$$

$$\rho(A) \propto A^{\alpha/2-1} \tag{2}$$

A simple method for α estimation is the box-gliding algorithm (Cheng, 1997). Define a set of square window sizes ε_i (ε_i=(2i−1)$\varepsilon_{\min}$, $\varepsilon_{\min} = < \varepsilon_1 < \varepsilon_2 \ldots < \varepsilon_i = \varepsilon_{\max}$, $i = 1, 2, \ldots, n$) for any given sampling point on the map. $\varepsilon_{\min}$ is the smallest window size, and $\varepsilon_{\max}$ is the largest window size. The density of element concentration ρ with in an area A of size ε_i can be acquired from the following power-law relationship:

$$\rho[A(\varepsilon_i)] = \frac{\mu[A(\varepsilon_i)]}{\varepsilon_i^{2}} = c\cdot\varepsilon_i^{\alpha-2} \tag{3}$$

where c is a constant. On the log-log plot, the relationship between $\rho[A(\varepsilon_i)]$ and ε_i can be fitted by least squares method, so as to determine the slop (α−2).

Most singularity indices with α≈2 satisfy normal or lognormal distributions, whereas the rest of singularity indices with extremely high and low values (α≠2) might follow fractal/multifractal distributions (Cheng, 2007; Cheng and Agterberg, 2009). For geochemical anomaly identification, singularity indices can be divided into three groups: (i) α-values < 2 indicate enrichment of geochemical concentration, being positive singularity; (ii) α-values > 2 indicate depletion of geochemical concentration, being negative singularity; and (iii) α-values closed to 2 indicate non-singular case. Therefore, estimation of singularity indices from a geochemical map can reflect different distribution patterns that might offer valuable information for mineral exploration.

2.2. Singularity-Quantile method

The S-Q method used for geochemical anomaly separation includes mutual transformations of the singularity indices between frequency domain and space domain. The key point of the method is how to appropriately process approximate values with α≈2.

In space domain, continuous singularity indices can be acquired by singularity analysis using box-gliding algorithm and interpolations such as inverse distance weighted (IDW) and multifractal IDW methods (Cheng, 2008), and then converted into frequency domain for statistical analysis. In frequency domain, the QQ-plot analysis is employed to detect the distribution patterns of singularity indices. As shown in Fig. 2, the x-axis is represented by the standard normal quantiles and the y-axis is represented by the quantiles of singularity indices. From a statistical point of view, the majority of values with α≈2 follow either normal or lognormal distributions (Cheng, 2007); we set the α-values that range from the 15th percentile to 85th percentile to determine the normal reference line. The normal distributed α-values will fall along or close to the normal reference line, and fractal/ multifractal distributed α-values will deviate from the normal reference line. Subsequently, the linear equation of normal reference line can be fitted by least squares method, meanwhile the residuals of fitting data can be obtained, locating on both sides of the normal reference line; further two linear equations can be acquired by fitting residuals. We set a 99% confidence interval of the singularity indices that pass through the 15th percentile and 85th percentile to limit the rangeability of the α-values. Another polynomial curve will be fitted by total α-values as shown in Fig. 2 with green color. Using these three equations, two intersection points or thresholds (x1, y1), (x2, y2) can be solved are located above and below the normal reference line, respectively (Fig. 2). Therefore, hybrid distribution patterns of singularity indices can be separated into three segments; then frequency-distributed singularity indices are converted back to spatial domain for visual representation of different geochemical anomaly populations. From the above demonstration on the method, we argue that the S-Q method provides insight into the nature of the geochemical anomaly from the fractal/multifractal and statistical points of view.

3. Case study

3.1. Geological setting

Geographically, the study area is located in the northwest of China attached to the southern margin of the Tianshan orogen, and to the north margin of the Xiemisitan belt; the east margin is Junggar basin and the west is bounded by Kazakhstan (Fig. 1a). Geologically, the study area belongs to the Central Asian Orogenic Belt (CAOB) that has