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A comparative study of trend surface analysis and spectrum–area multifractal model to identify geochemical anomalies

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ABSTRACT

The trend surface analysis (TSA) and the spectrum–area (S–A) multifractal model are two popular methods to identify geochemical anomalies. In this study, the robust principal component analysis (RPCA) was applied to integrate multi-geochemical variables in a regional stream sediment dataset related to major ore-forming elements in southwestern Fujian (China). We applied the TSA and S–A model to decompose the integrated geochemical pattern obtained from the RPCA and compared the results obtained from both methods. The obtained anomaly maps were similar, with the high anomaly areas showing a strong spatial relationship with intrusions that are related to Fe polymetallic mineralization, indicating that both the TSA and the S–A are useful tools to identify geochemical anomalies. The S–A model, based on distinct anisotropic scaling properties, was better in revealing local anomalies because it considered the spatial characteristics of the geochemical variables.

1. Introduction

A fundamental task in geochemical exploration is the separation of background patterns from geochemical anomalies, which are the direct consequences of coupled physical and chemical processes occurring within the upper crust of the Earth, due to various different geological processes, leading to different mineralization types (Cheng, 1999; Zhao et al., 2009; Zhao, 2014). To simulate the coupled physical and chemical processes involved in ore-forming systems, the emerging computational geoscience methods have been developed in recent years through extensive and systematic research (e.g., Zhao, 2015; Zhao et al., 2009, 2014b).

From the scientific point of view, an ore-forming system can be treated as a nonlinearly-coupled mathematical problem involving dynamic interactions between rock deformation, pore-fluid flow, heat transfer, mass transport and chemical reaction processes (Alt-Epping and Zhao, 2010; He et al., 2013; Hobbs et al., 2000, 2010; Liu et al., 2011; Poulet et al., 2013; Schmidt Mumm et al., 2010; Zhao et al., 2009). This kind of nonlinear coupled problem can cause thermodynamic instability (e.g., Hobbs et al., 2004, 2007; Zhao et al., 1998, 2012), and physical and chemical dissolution-front instability (e.g., Hobbs et al., 2008; Zhao et al., 2010, 2013), which are the main dynamic mechanisms that control the formation of anomalous patterns in ore-forming systems. Accurate simulation of these coupled processes is the goal of emerging computational geoscience methods, which have been widely employed to predict ore distribution patterns to assist mineral exploration (Hobbs et al., 2000, 2010; Liu et al., 2011; Schmidt Mumm et al., 2010; Zhao et al., 2009, 2014a).

On the other hand, early quantitative methods and techniques such as probability graphs, mean, and percentiles have been developed for identification of geochemical anomalies based on a constant geochemical threshold (Miesch, 1981; Sinclair, 1974, 1991; Stanley and Sinclair, 1989). However, different subareas can differ in rock composition or have experienced different geological processes, which results in different geochemical thresholds. Therefore, these methods are not adequate to identify weak geochemical anomalies since many may be lost because of geochemical background variation. In this study, TSA and S–A model were compared based on a case study from southwestern Fujian Province (China).

2. Methods

2.1. Robust principal component analysis

The principal component analysis (PCA) is one of the most popular methods of multivariate data analysis (e.g., Carranza and Hale, 1997; Cheng, 2011; Rubio et al., 2000). The PCA converts high dimensional data to a lower dimensional space based on a covariance or correlation matrix. The main aim of the PCA is to explain as much data information as possible from the least uncorrelated (principal) components. However, geochemical data usually contain outliers and are heterogeneous. The classical estimators (e.g., arithmetic mean, sample covariance matrix) are sensitive to outliers, severely affecting the classical PCA results, and rendering them meaningless (Filzmoser et al., 2010; Locantore et al., 1999). Robust statistical approaches can resist some contamination, which focus on the main data structure and reduce the influence of

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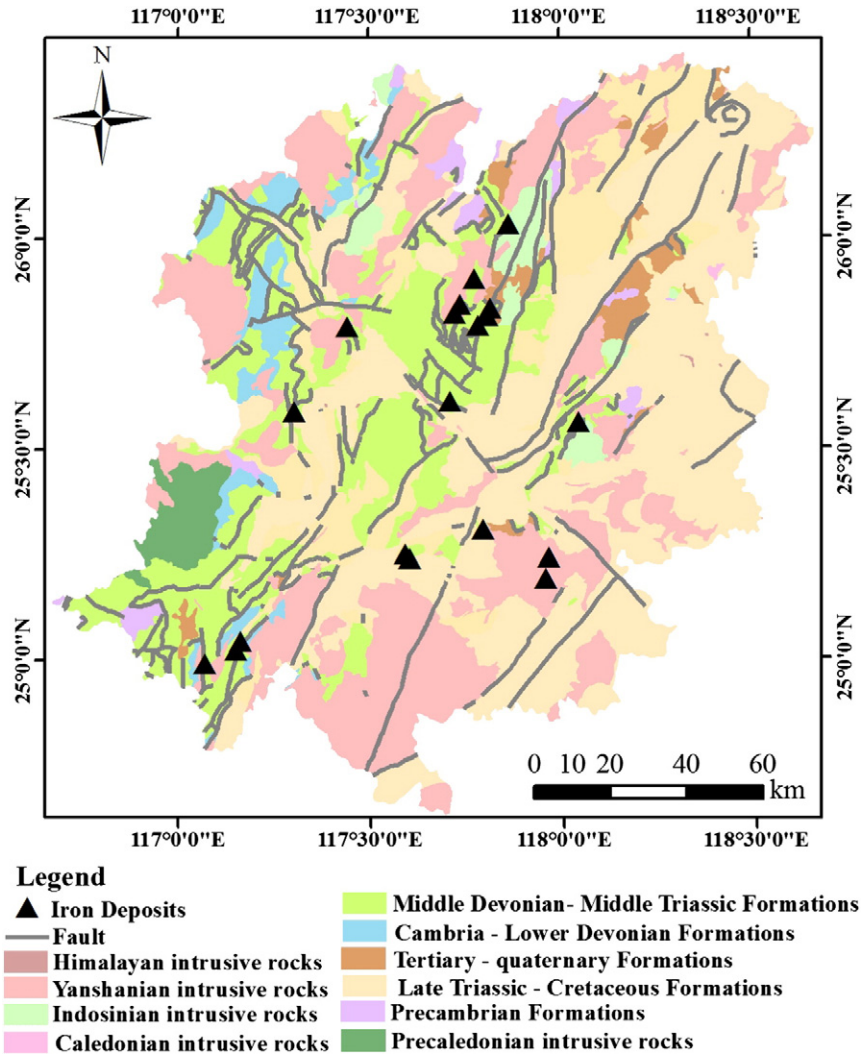

Fig. 1. Simplified geological map of the southwestern Fujian province in China (modified from Fujian Geology & Mineral Exploration Bureau, 2011).

outliers. The robust PCA (RPCA) based on minimum covariance determinant (MCD) estimator has become popular (Rousseeuw and Driessen, 1999).

In addition, geochemical data are typically compositional data, in the form of some proportions such as weight percent, parts per million, etc., subject to a constant sum (e.g., 100%, 1,000,000 ppm). RPCA only applies to Euclidean space, indicating that compositional data based on simplex geometry needs to be transformed by logratio transformation prior to the RPCA (Aitchison, 1986; Aitchison et al., 2000; Carranza, 2011; Egozcue et al., 2003; Filzmoser and Hron, 2008; Reimann et al., 2012). There are three popular logratio transformation methods for opening the compositional data: additive logratio transformation (***alr***) (Aitchison, 1986), centered logratio transformation (***clr***) (Aitchison, 1986), and isometric logratio transformation (***ilr***) (Egozcue et al., 2003). In this study, the ***ilr*** was used to process the raw geochemical data because of the isometry between the simplex and the Euclidean spaces, so that the statistical methods were suitable for processing ***ilr***-transformed data. For a geochemical composition X in the D-part simplex S^D, the ***ilr*** gives (Egozcue et al., 2003):

$$y_i = \sqrt{\frac{D-i}{D-i+1}} \log \frac{x_i}{\sqrt[D-i]{\prod_{j=i+1}^{D} x_j}} \qquad i = 1, 2, 3, \ldots, D-1. \tag{1}$$

2.2. Trend surface analysis

The TSA, based on the least-sum-of-squares, aims to fit mathematical surfaces of increasing complexity to a variable distributed on a map (Oliveira, 1979). It has become a popular technique to separate spatial patterns into two components: a regional trend and residual values (Agterberg, 1974; Davis and Sampson, 2002; Unwin, 2009). The regional trend, regarded as the geochemical background, is computed by polynomial surfaces of successive powers; while the residual values, corresponding to geochemical anomalies, are the arithmetic differences between the original data and the trend surface, indicating local fluctuations. Residual maps are associated with local features of interest.

A trend map delineates the general distribution of an element, and the local variations are emphasized after the removal of systematic variations (Nichol et al., 1969). The trend surface function gives (Oliveira, 1979):

$$z_i(x_i, y_i) = \hat{z}_i(x_i, y_i) + \varepsilon_i \tag{2}$$

where $z_i(x_i, y_i)$, $_i(x_i, y_i)$, and ε_i are the observed, trend, and residual values of variable Z at location (x_i, y_i). ε_i represents the small-scale fluctuations plus a random error component. The unknown parameters