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Research paper

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

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A R T I C L E I N F O

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A B S T R A C T

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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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, ..., 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

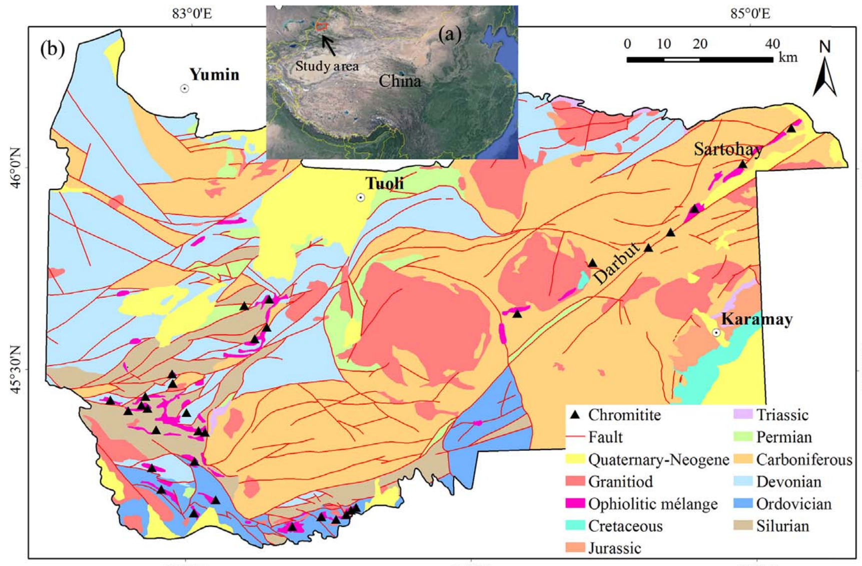

Fig. 1. (a) The location of the study area, (b) simplified geological map of the western Junggar region, China.

experienced complicated collision and accretion processes during the evolution of the Phanerozoic accretionary orogens (e.g., Sengör et al., 1993; Chen and Arakawa, 2005; Xiao et al., 2008). The main rock assemblages include Carboniferous, Silurian and Devonian sedimentary formations, Carboniferous granitoid intrusions, and Paleozoic ophiolitic mélanges (Fig. 1b). The Carboniferous sedimentary formations and ophiolitic mélanges are regionally intruded by Carboniferous granitoid intrusions (Chen and Arakawa, 2005; Chen et al., 2014). The Devonian sedimentary formations are composed of basalt lavas interbedded with chert and some volcanic rocks. The most striking geological feature is the outcrop of many ophiolitic rocks, principally serpentinite, located along the Permian high-angle strike-slip fault zone across the western Junggar region (Allen et al., 1995; Chen et al., 2014). Structurally, a series of NE-trending faults were developed in the western Junggar region. The western Junggar is one of the most important chromitite metallogenic belts in China. Up to now, many chromitite deposits have been discovered, of which Sartohay is the largest chromitite deposit formed in the mantle peridotite of the Sartohay ophiolitic mélange (Hao et al., 1990). Most of the chromitite mineralization occurred in harzburgite, surrounded by dunites, containing well-preserved mantle-derived peridotites, which are the end products of larger-scale mantle processes (Shi et al., 2012; Tian et al., 2015).

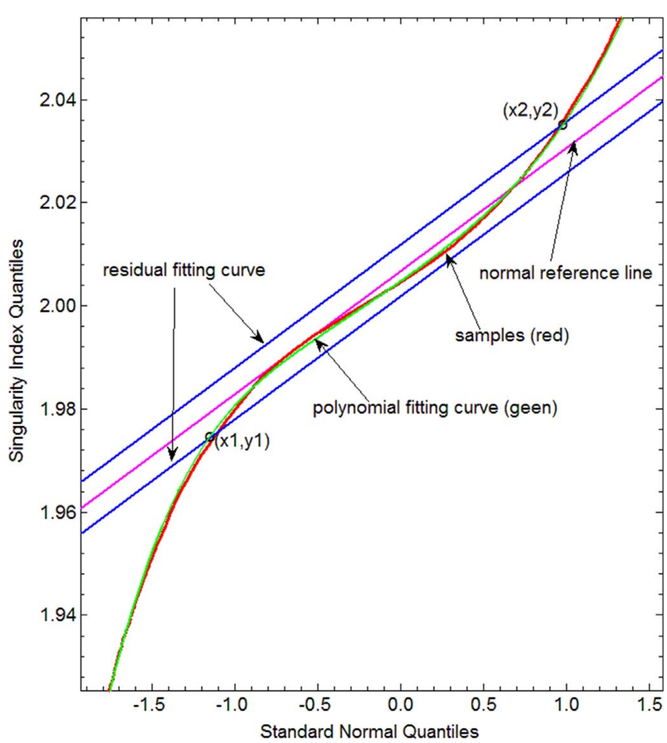

Fig. 2. Illustration of S-Q method in frequency domain.

3.2. Data used

Total of 4814 stream sediment samples have been collected with a density of around one sample per 4 km^2. Details of sample collection and chemical analytical methods of stream sediments can be found in Xie et al. (1997) and Liu et al. (2016). Data used in the case study include 18 geochemical elements (Mo, Ni, Ag, Co, Cr, Cu, Mn, Pb, As, Au, Ti, Zn, K, Mg, Sb, Na, Si, and Al), of which K, Mg, Na, Si, and Al are expressed by their oxides.

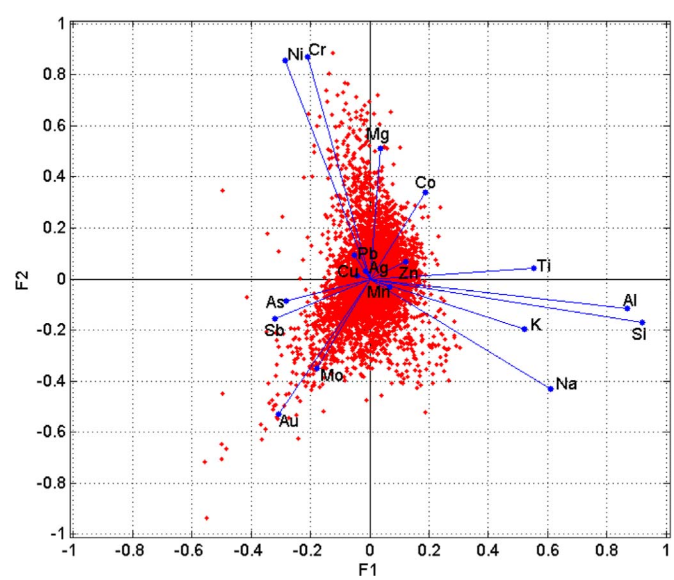

Fig. 3. Biplot of F1 vs. F2 derived from the CoRFA method.

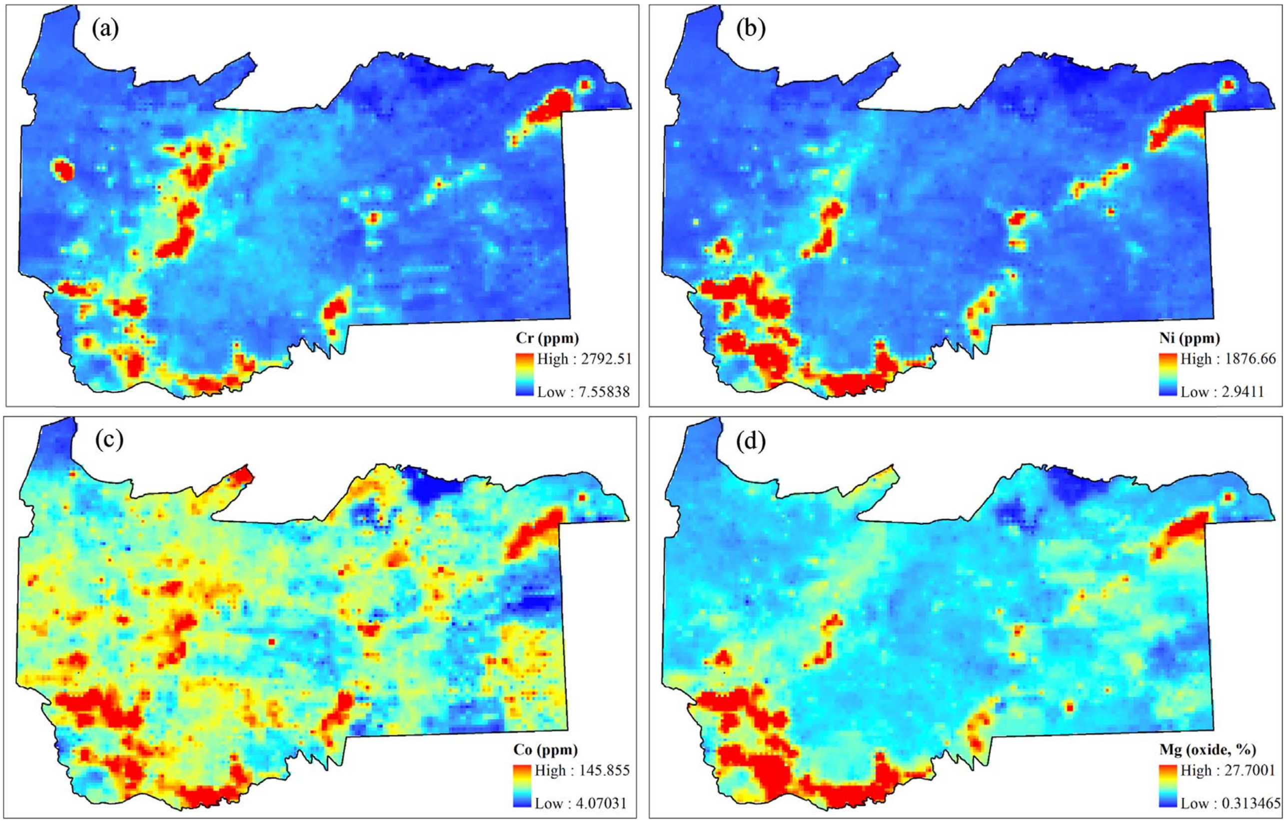

Fig. 4. Spatial distribution of four geochemical elements mapped by IDW interpolation (a) Cr, (b) Ni, (c) Co, and (d) Mg.

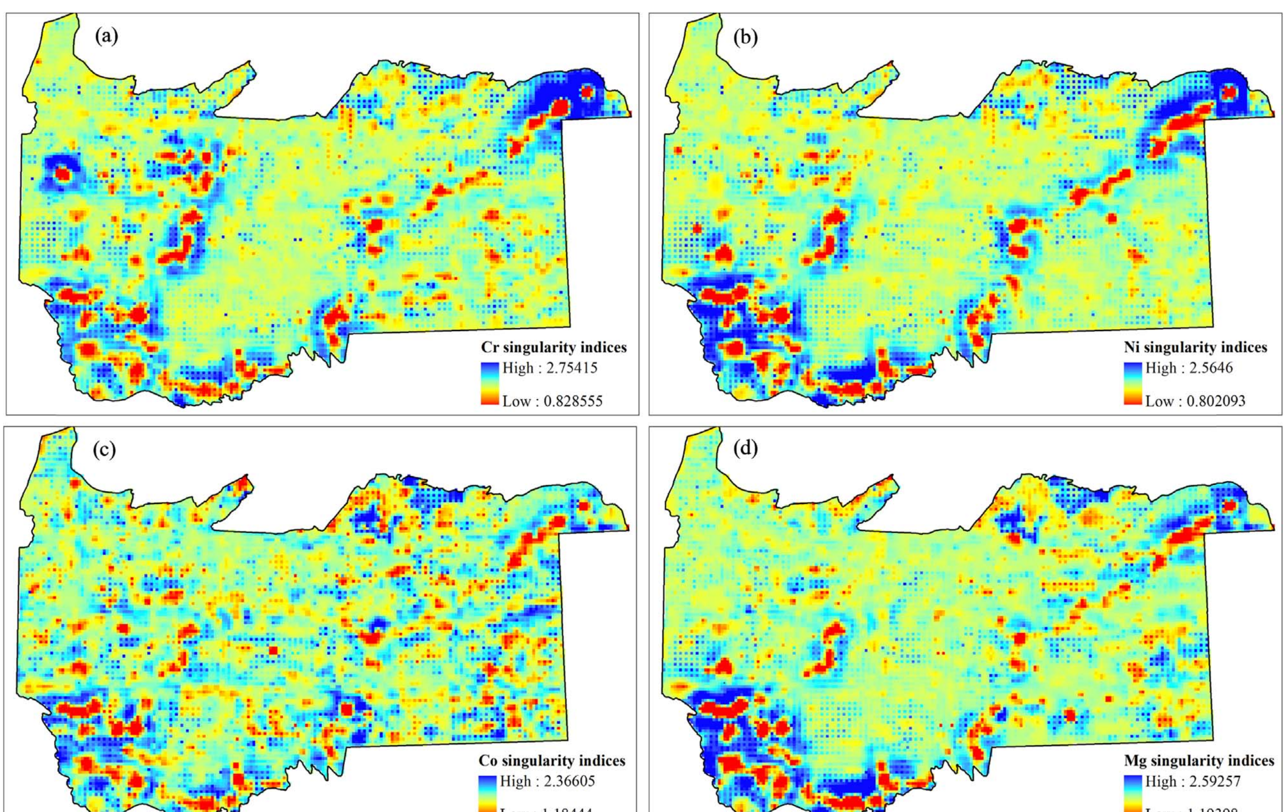

Fig. 5. Singularity maps with continuous values of (a) Cr, (b) Ni, (c) Co, and (d) Mg.

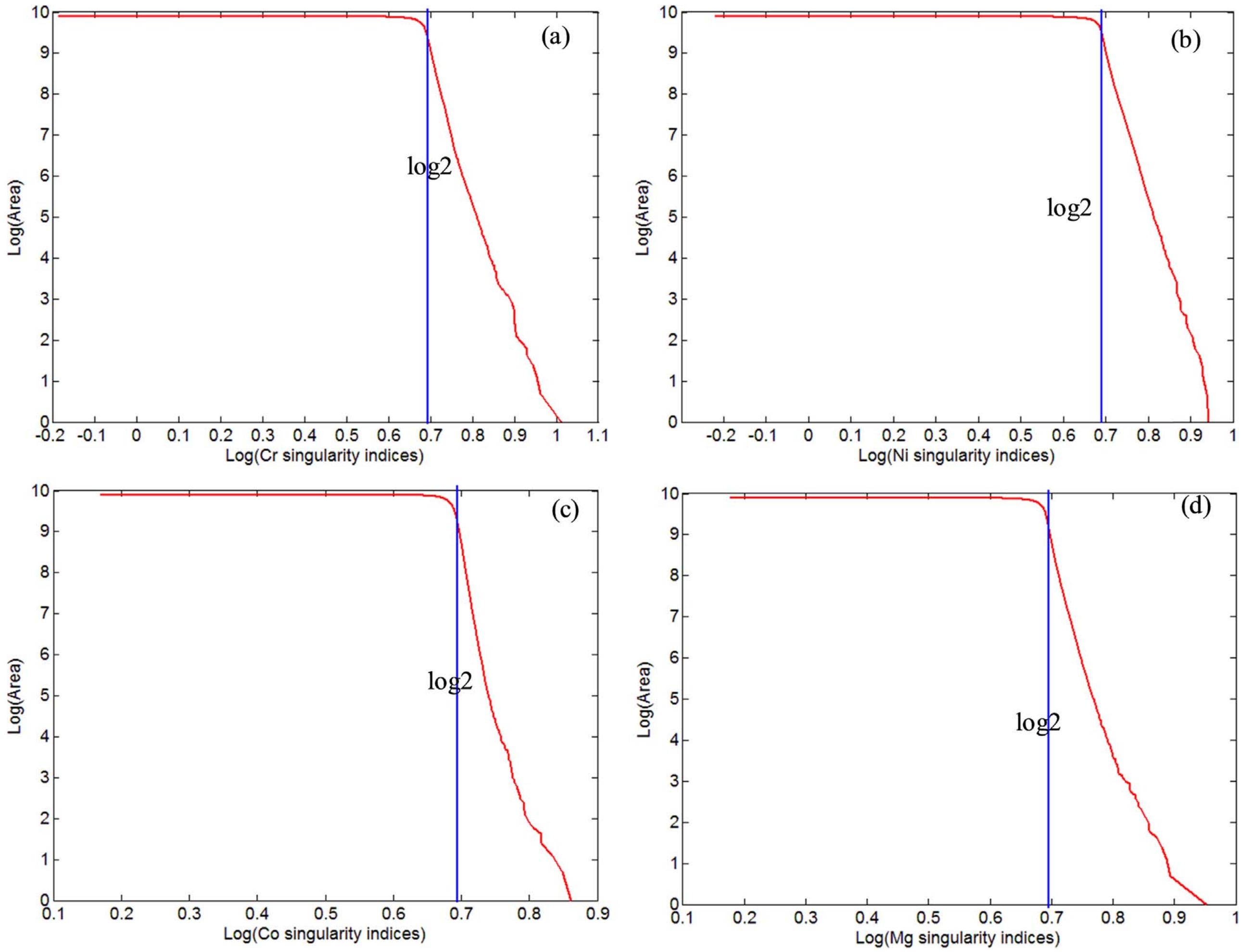

Fig. 6. C-A plots based on singularity indices of (a) Cr, (b) Ni, (c) Co, and (d) Mg.

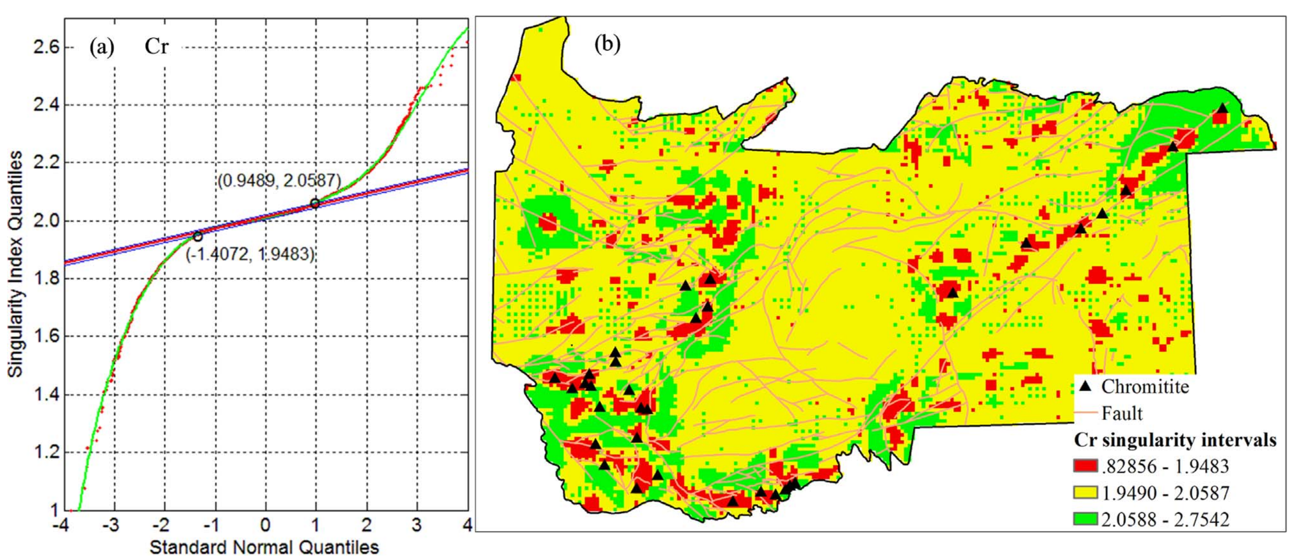

Fig. 7. (a) Cr singularity index quantiles vs. standard normal quantiles, and (b) singularity map with categorical values based on S-Q analysis. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

3.3. Determination of chromitite mineralization-related geochemical elements

Geochemical data are commonly considered as compositions, expressed in weight percent or parts per million/billion (e.g. 100%, ppm, wt%) and subject to the influence of a constant sum (Aitchison, 1986; Pearson, 1897; Carranza, 2011; Egozcue et al., 2003). In order to reduce the influences of data closure and outliers, a compositional robust factor analysis (CoRFA) was performed to study potential correlations associated with chromitite mineralization among 18

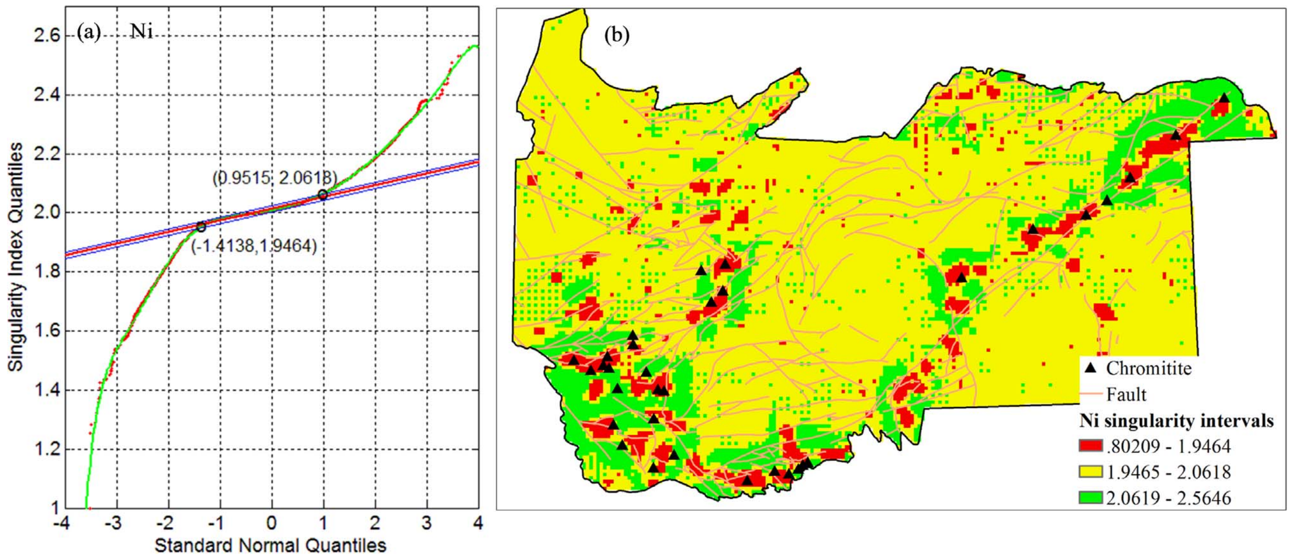

Fig. 8. (a) Ni singularity index quantiles vs. standard normal quantiles, and (b) singularity map with categorical values based on S-Q analysis. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

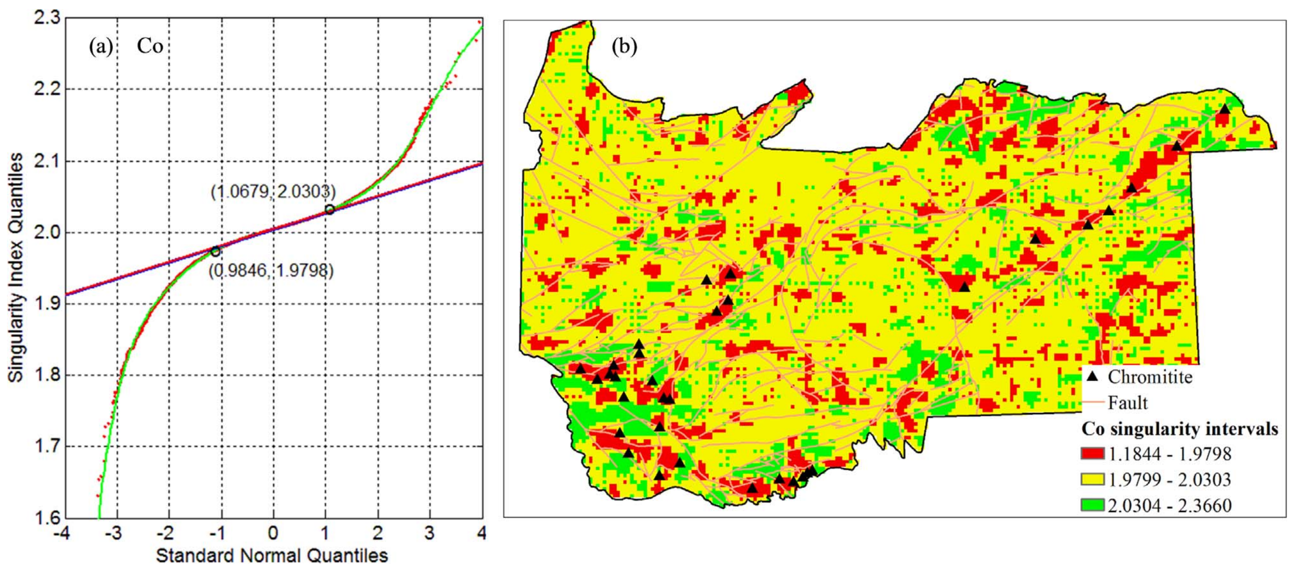

Fig. 9. (a) Co singularity index quantiles vs. standard normal quantiles, and (b) singularity map with categorical values based on S-Q analysis. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

geochemical elements in the western Junggar region (China). Major steps of the CoRFA method include (Liu et al., 2016): (1) transformation of geochemical data by using of centered log ratio (clr) method; (2) application of the minimum covariance determinant (MCD; Rousseeuw and Driessen, 1999) to estimate the robust covariance matrix based on isometric log ratio (ilr) transformed geochemical data; (3) back-transformation of ilr coordinates to clr coefficients by means of an orthonormal basis (Egozcue et al., 2003); (4) robust covariance matrix for clr coordinates estimated from the relationship between clr and ilr, and used to determine robust correlation matrix; (5) Initial factor loading and common variance obtained by factor rotation and singular value decomposition (SVD) of correlation matrix. Rotation factor loadings can be operated by orthogonal (e.g., Varimax) and oblique (e.g., Promax). In the present study, the Promax method is considered, since it provides better interpretation of underlying relationships among geochemical elements.

The first three factors account for 52.4% of the total variance, of which the first factor (F1) accounts for 26.7%. The biplot of F1 vs. F2 (Fig. 3), indicates that three types of multi-elemental associations can be recognized. The positive F1 contains an association mainly composed of Si, Al, Na, K, and Ti; the negative F2 reflects an association of Au, Mo, As, and Sb; and the positive F2 reflects an association of Cr, Ni, Co, and Mg. It should be noted that F1 includes mixed information, trying to explain as much information as possible, while subsequent factors commonly reflect specific processes (Liu et al., 2016). Based on the results of the CoRFA, favorable geochemical elements including Cr, Ni, Co, and Mg that are closely associated with chromitite mineralization can be determined objectively.

3.4. Singularity-Quantile method for separating geochemical anomaly populations

For further comparison with the results obtained from the S-Q method, the spatial distribution of Cr, Ni, Co, and Mg were mapped by the IDW method with searched minimum number of samples equal to 12 (Fig. 4). Then, singularity analysis was employed to measure the intensity of enrichment or depletion of each element at different locations. Singularity indices of Cr, Ni, Co, and Mg were respectively

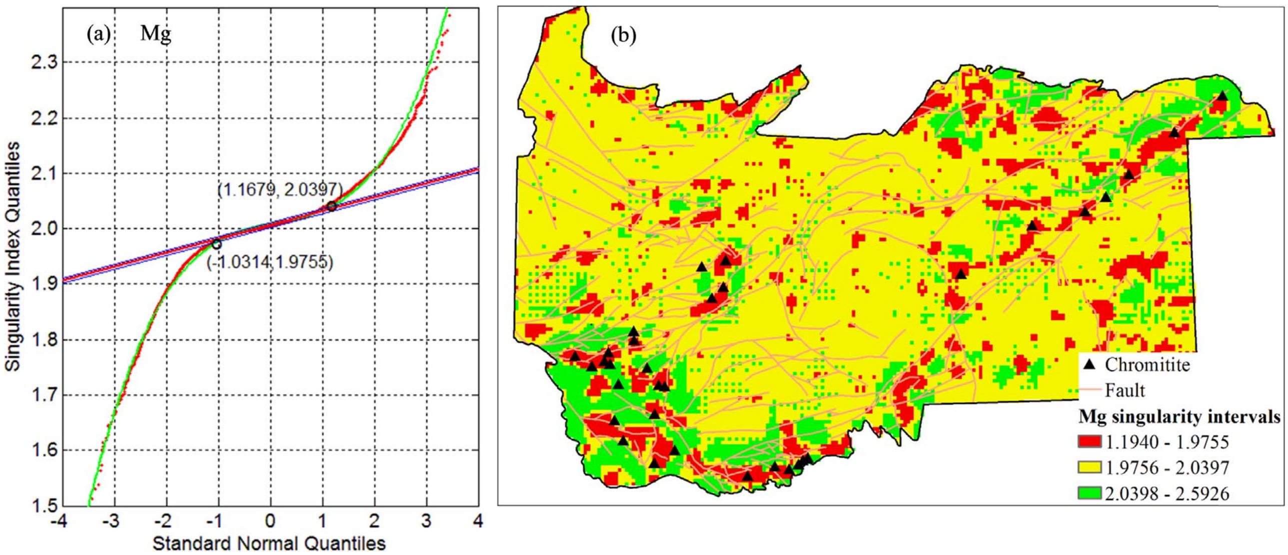

Fig. 10. (a) Mg singularity index quantiles vs. standard normal quantiles, and (b) singularity map with categorical values based on S-Q analysis. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Table 1
The area percentage of four elements' singularity indices with α<2, α≈2, and α>2.

Elements	Area percentage of singularity indices		
	α<2	α≈2	α>2
Cr	8.42%	74.30%	17.27%
Ni	7.48%	75.60%	16.92%
Co	16.08%	70.29%	13.63%
Mg	13.37%	71.98%	14.65%

estimated by means of the box-gliding algorithm with thesquare window sizes ε_i ranging from 3, 5, 7, ..., to 15 (Fig. 5). The result shows that local weak and concealed geochemical anomalies were enhanced by singularity analysis compared with the original element concentration maps (Figs. 4–5).

In order to distinguish different geochemical anomaly populations, Liu et al., (2013, 2014b) combined singularity analysis and C-A method to delineate three types of geochemical anomalies, corresponding to high anomalous, moderate anomalous and low anomalous zones, respectively. However, in the present case study, it seems hard to detect two suitable thresholds on the curves with three types of geochemical anomalies when the C-A method was performed on singularity indices, because intensive changes of curve slope occurred around the value of log2 (0.693), as indicated by Fig. 6.

As demonstrated in Section 2.1, singularity indices (α-values) can characterize different geochemical distribution patterns such as normal and multifractal distributions. For our case study, the distribution patterns of singularity indices were clearly distinguished by the S-Q method in frequency domain, as indicated by Figs. 7a–10a. Actually, the α-values above and below the fitting lines satisfy fractal/multifractal distributions, corresponding to element depletion and element enrichment, respectively; while α-values close to 2 limited by the two fitting lines satisfy normal distributions, corresponding to element generality or geochemical background. Two intersection points (thresholds) can be easily calculated by solving linear and polynomial equations, and three geochemical anomaly populations were separated graphically (Figs. 7a–10a).

Based on the thresholds, singularity indices of Cr, Ni, Co and Mg were projected into space domain with three partitions shown in

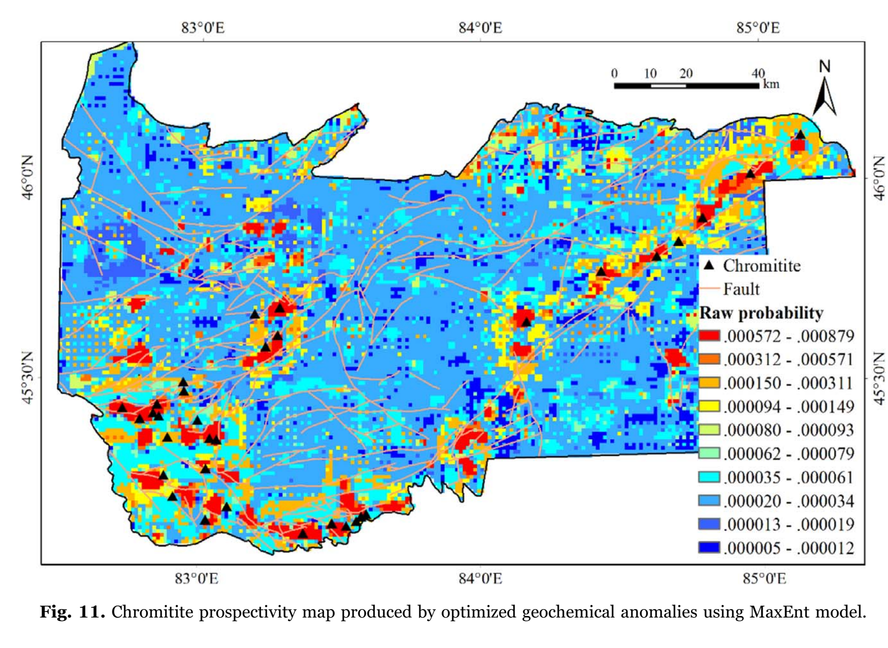

Fig. 11. Chromitite prospectivity map produced by optimized geochemical anomalies using MaxEnt model.

Figs. 7b-10b. Table 1 shows areas with non-singular geochemical data of each element accounting for more than 70% of the study area; areas with element enrichment or depletion of individual elements occupy smaller percentage of the study area. As shown in Figs. 7b-10b, the red color represents favorable zones for chromitite mineralization delineated by $\alpha < 2$, and the blue color represents unfavorable zones for chromitite mineralization delineated by $\alpha > 2$. Obviously, the scope for discovering potential chromitite mineralization is reduced greatly by means of the S-Q method. The results also indicate that geochemical anomaly populations are of distinct zoning features in space domain that can be observed in the southwest parts of the study area and along the Darbut fault zone (Figs. 7b–10b), where areas with element enrichment are located in the center, outside of which are element generality zones, and the outmost parts are element depletion zones.

3.5. MaxEnt model for geochemical anomaly optimization

The MaxEnt model is a machine learning method with a very flexible algorithm has been fully described by Phillips et al. (2006) and Phillips and Dudík (2008). Although the model has been widely used for predicting species distribution in the field of ecology (Elith et al., 2006; Pearson et al., 2007), its applicability to mineral potential mapping has been seldom reported. In order to optimize different geochemical anomaly populations derived from the S-Q method for chromitite prospectivity analysis from a geochemical data point of view, the MaxEnt model was used to produce chromitite prospectivity map aided by Maxent software (https://www.cs.princeton.edu/~schapire/maxent/). Four categorical singularity maps with three classes of Cr, Ni, Co and Mg were integrated in the model (Figs. 7b–10b). The tough problem of the MaxEnt model is overfitting, which can be constrained by the so called β-regulation (Elith et al., 2011). However, the results of the case study were almost unaffected by model overfitting by examination of β-regulation, since fewer input variables were used, and that were categorical variables. Therefore, the defaulted settings for feature type, raw output, and regularization in the Maxent software was used for chromitite prediction. The model successfully linked multiple geochemical anomaly populations derived from S-Q method with known chromitite locations. The chromitite prospectivity map shows that most of the chromitite locations are spatially consistent with element enrichment zones marked in red colors (Fig. 11). Therefore, the prospectivity map can considered as an important guidance for predicting the locations of concealed chromitite deposits from the multifractal point of view.

4. Conclusions

In the present study, the S-Q method based on integrating singularity analysis and QQ-plot analysis is investigated to separate multiple geochemical anomaly populations by determination of reasonable thresholds. The method considers the frequency and space distribution patterns of singularity indices. In frequency domain, geochemical distribution patterns of singularity indices can be separated into three populations based on plotting the singularity index quantiles vs. standard normal quantiles, corresponding to element enrichment, element generality and element depletion, respectively. The S-Q method provides us reasonable explanation from the statistical and multifractal points of view in terms of geochemical anomaly identification and separation.

Statistically, the QQ-plot analysis is a graphical method for comparing two probability distributions by plotting their quantiles against each other. Commonly used normal QQ-plot analysis functions such as the *qqplot* in MATLAB software and the *qqnorm* in R environment (http://www.astrostatistics.psu.edu/su07/R/html/stats/html/qqnorm.html), cannot be directly performed to separate multiple populations of singularity indices at a 99% confidence interval of the fitting residuals, because the normal reference line is produced by joining the first quartile (25^{th} percentile) and third quartile (75^{th} percentile) of each distribution. The QQ-plot analysis as an exploratory data analysis (EDA) method, for our studies the normal reference line produced by passing through the 15^{th} percentile and 85^{th} percentile of the singularity indices was adopted, since an excellent result can be captured by using of a 99% confidence interval of the fitting residuals.

A case study for chromitite prospectivity analysis based on geochemical data in western Junggar region(China), was employed to examine the potential application of the proposed method. Preliminary data analysis is important, in order to obtain more objective results. In the case study, the CoRFA method was performed to determine which geochemical elements are closely related to chromitite mineralization. The results revealed that the S-Q method can efficiently recognize and partition hybrid geochemical anomaly populations, because the method is very sensitive to the changes of singularity indices with three segments when it was applied to characterize the geochemical element enrichment processes. In order to optimize different geochemical anomaly populations of individual variables, the MaxEnt model was employed to generate chromitite prospectivity map, indicating that the optimized geochemical anomalies can efficiently delineate chromitite-related mineralization and largely reduce chromitite exploration areas.

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