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Exploratory data analysis and singularity mapping in geochemical anomaly identification in Karamay, Xinjiang, China

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ABSTRACT

Hatu and Baogutu are two typical gold deposits in the study area. Hatu gold deposit is associated with magmatism and controlled by regional-scale faults; mineralisation mainly occurs within hydrothermally altered felsic rocks and quartz veins. In the west region of the Hatu mining area, Cu, Ag, As and Sb are present in high concentrations in carbon tuffaceous shale. Baogutu gold deposit is associated with the evolution of felsic magmas, and the porphyry copper-gold mineralisation and copper-gold ore body dominated by sulphide were formed in the rock or near the contract zone in the faults, respectively. The ore-forming elements include Au, As and Sb. In this study, exploratory data analysis (EDA) and singularity mapping (SM) techniques were applied to identify geochemical anomalies caused by Au-related mineralisation according to stream sediment geochemical data set in Karamay mineral district, northwestern China. Silver, As, Au and Sb were chosen as indicator elements. The results show that EDA could not well identify weak anomalies within the strong variance of the background, while SM can recognise effectively weak anomalies, and quantify the properties of enrichment caused by mineralisation. The results obtained by SM demonstrated that the anomalies are closely associated with the known Au deposits in the study area. The anomalous areas delineated by the SM have potential for follow-up mineral exploration. In addition, the results document that Ag, As, Au and Sb may be reliable indicator elements for Au-related mineralisation in the study area.

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1. Introduction

Identifying anomalies during mineral exploration is one of the basic tasks in geochemical data utilisation. Several techniques can be used to identify anomalies in geochemical data sets, which can be broadly classified into two categories according to the number of thresholds used in the study area: (i) 'hard threshold techniques' (employing a global threshold level for all data in the study area), and (ii) 'soft threshold techniques' (which employs local, dynamical thresholds over a study area). For hard threshold techniques, the anomaly threshold is often calculated, e.g. by using the mean of a variable or element plus two or three times the variable/element's standard deviation (MSTD) (Reimann and Garrett, 2005; Reimann et al., 2005; Xie et al., 2008a), or by the value of the median of a variable or element plus two times the median absolute deviation (MMAD) (Bounessah and Atkin, 2003; Chipres et al., 2009; Reimann and Filzmoser, 2000; Reimann et al., 2005) or by using the concentration–area (C-A) multifractal model (Cheng et al., 1994). In soft threshold techniques, some window-based contrast filtering methods (Jin and Chen, 2011; Shi et al., 1999; Zhao et al., 2012b), such as the spectrum and area model (S-A model) (Cheng, 2000) and the SM technique developed by Cheng (2007a), are widely used (Chen et al., 2007; Cheng et al., 2009; Wang et al., 2013a, b; Zuo and Cheng, 2008; Zuo et al., 2013, 2015–in this issue).

In China, the MSTD is often used as the canonical anomaly threshold definition, in the statistical treatment of regional geochemical data for mineral exploration, even at the present time when computers and new and efficient techniques are available. MMAD, as a kind of exploratory data analysis (EDA), is considered a *robust* method of treating exploration data. By contrast, the C-A model has limited success in identifying weak anomalies in covered areas (Zuo et al., 2013), and expert knowledge is needed to determine the anomaly threshold according to the log-log plot. The problem in using contrast filtering methods is that the size of the window used needs to be determined according to *a priori* knowledge, which limits practical application. The S-A model is complicated and suffers from edge effects in irregularly shaped study areas (Zuo et al., 2013). By contrast, the SM technique has been reported widely and often produces meaningful results when used in the statistical treatment of geochemical data (Bai et al., 2010; Cheng, 2012; Sun et al., 2010; Xiao et al., 2012; Zuo et al., 2013).

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In this paper, the Hatu and Baogutu gold districts in Karamay, Xinjiang, China are selected as the study area used for comparison of the results of MMAD (hard threshold) and the SM technique (soft threshold) with respect to identifying geochemical anomalies associated with mineralisation.

2. Study area and data set

The study area (Fig. 1) is located in the western Junggar Basin, approximately 330 km northwest of Urumqi, Xinjiang, China. This district is mainly controlled by NNE faults. Major faults in this area include, from north to south, the Hatu, Anqi, Darabut and Yijiaren faults. The Darabut ophiolitic mélange belt, distributed as a band along the Darabut fault, is approximately 50 km^2 in size, which was tectonically disrupted, and now forms the present imbricate structure that is mainly controlled by thrust faults. Materials from the oceanic crust often appear in terrigenous detrital sediment at old continental margins, and exhibit geochemical characteristics that are similar to the materials from the mantle (Zhang and Huang, 1992). Major plutonic rocks are represented by Miaoergou, Hatu, Akebasitao, Red Mountain and north Karamay granite batholiths in this area, with an age of 300 Ma from zircon LA-ICP-MS U-Pb (Su et al., 2006). The distributions of intrusive rocks and ore deposits in this area are highly correlated with the faults.

The Hatu gold deposit in the NW and the Baogutu gold deposit in the SE of the study area are two representative deposits of the regional mineralisation geology. The Hatu gold deposit is controlled by two NE trending faults, namely, Anqi (extension fault) and Hatu (compression and scissor fault). Some NW, NE and EW trending secondary faults are associated with ore formation and with the NE trending fault. The ore bodies occur in groups, en échelon, and end-to-end alignment (Zhu et al., 2013). The Hatu gold deposit mainly consists of superficial quartz vein-type and altered rock-type ore bodies, and these ore bodies are products of a homologous hydrothermal flow (Zhang, 2003). Copper, Ag, As and Sb are present in high concentrations in carbon tuffaceous shale. Antimony occurs in the Lower Carboniferous stratum. Gold mineralisation is associated with silicification, sericitisation, pyritisation and arsenopyrite mineralisation. The main mineral assemblage is arsenopyrite-pyrite-native gold-native arsenic-native antimony-stibnite. Arsenopyrite is the ore mineral of this gold deposit, and its element association is Au, As and Sb (Zhu et al., 2013).

China's National Geochemical Mapping Project (Regional Geochemistry National Reconnaissance) was initiated in 1979 (Xie et al., 1997), and the project covered more than 6 million km^2 (Xie et al., 2008b). This project mainly collected stream sediment samples. In this study, the density was one sample per km^2. To reduce the laboratory load, four samples were composited into one sample for analysis representing 4 km^2 (Fig. 2). For the purposes of this study, four elements were selected from the 39 elements that were determined (Wang et al., 2011; Xie et al., 2008b), which are closely related to the mineralisation, namely, Ag, As, Au and Sb. Silver was determined using emission spectrometry (ES) with a detection limit of 0.1 mg/kg. Arsenic and Sb were determined by hydride generation–atomic fluorescence spectrometry (HG-AFS), and their detection limits were 0.005 and 0.1 mg/kg respectively. Gold was determined by graphite furnace–atomic absorption spectrometry (GF-AAS) with a detection limit of 0.1 mg/kg. Details on the quality control procedures are reported by Xie et al. (1996), Cheng et al. (1997) and Liu et al. (2015–in this issue).

Many research projects on geochemical anomaly recognition were conducted on the basis of China's National Geochemical Mapping Project, and these projects used methods such as the C-A fractal model (Cheng et al., 1994), the concentration–distance fractal model (Li et al., 2003), the spectrum–area (S-A) model (Cheng, 2000), and the SM technique (Cheng, 2007a; Wang et al., 2013b; Xiao et al., 2012; Zuo et al., 2009, 2012, 2013), which involved both the frequency distributions and the spatial self-similar properties of geochemical variables. These models are effective tools for decomposing complex and mixed geochemical populations, and for identifying weak geochemical anomalies hidden within a strong geochemical background (Cheng, 2007a; Cheng and Agterberg, 2009; Cheng et al., 2010). In the present paper, the effectiveness of EDA and SM techniques to identify geochemical anomalies related to gold deposits are compared using the stream sediment geochemical data from the Karamay area.

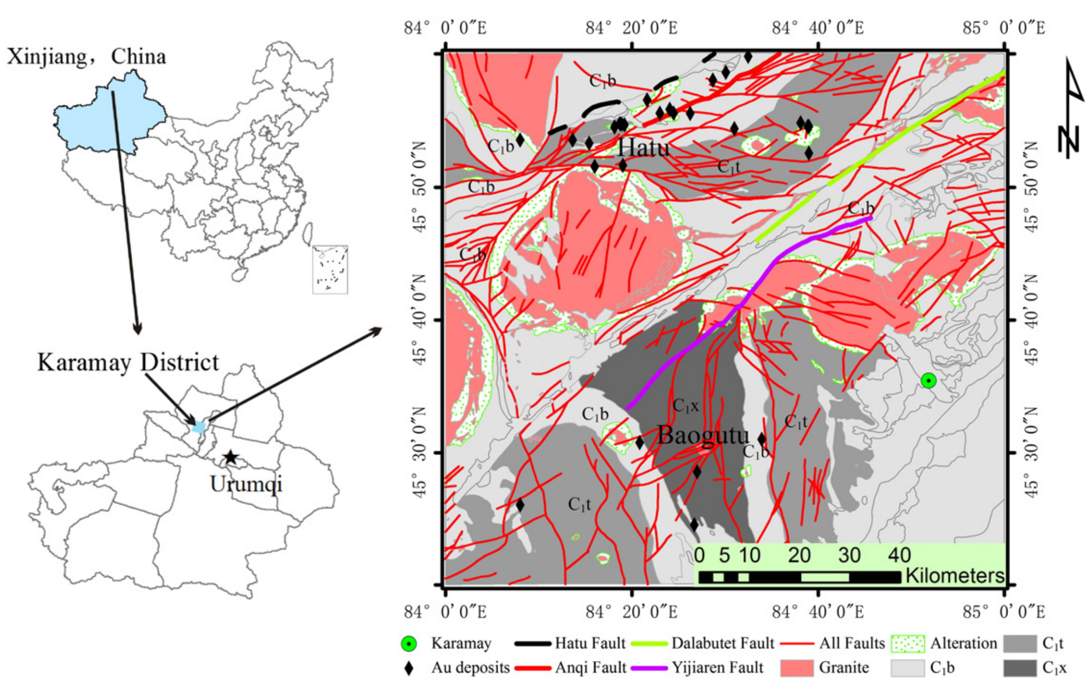

Fig. 1. Simplified map of regional tectonics, magmatic rocks and alteration districts in the northwestern Xinjiang Autonomous Region, China (C1x = Xibeikula formation; C1t = Tailegula formation; C1b = Baogutu formation).

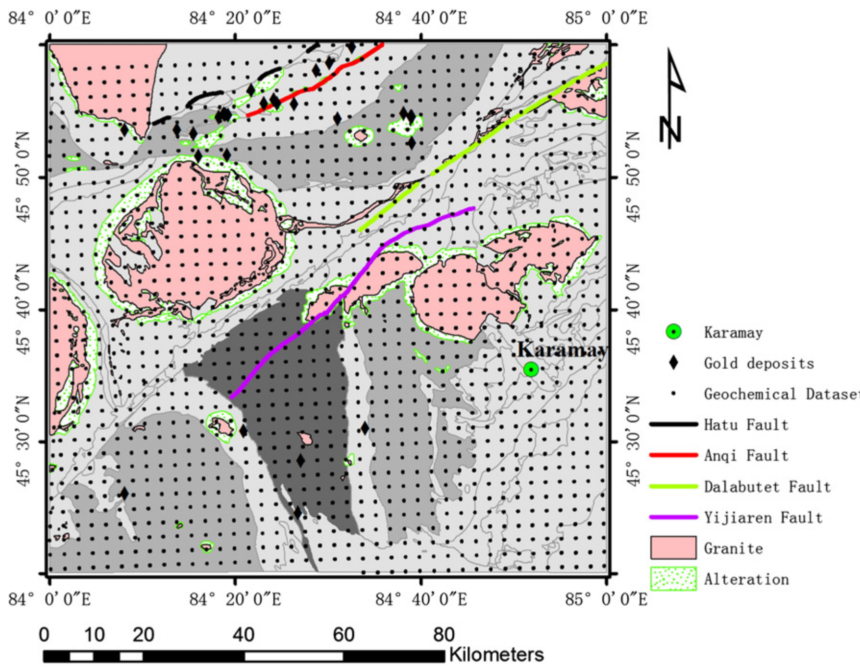

Fig. 2. Simplified map of stream sediment geochemical sample locations.

3. Methodology

3.1. EDA

The principles of the EDA (Tukey, 1977) are unlike those of conventional statistical techniques because EDA does not require a data set to follow normal or log-normal distribution. A boxplot is plotted by first ordering data values from minimum to maximum, or vice versa (Kürzl, 1988). The median value is determined by counting halfway through the data values, thereby dividing the univariate data set into two equal parts. Subsequently, by counting halfway from the minimum to the median and from the maximum to the median, the lower hinge (LH) and the upper hinge (UH) values are estimated, respectively. With the lower hinge, median and upper hinge, a data set is thus divided into four approximately equal parts known as quartiles. A box is then drawn between the lower and upper hinges. The box is usually divided by a line at the median value. The absolute difference between the values at the lower and upper hinges represents the inter-quartile range (IQR) or hinge width:

$$\text{hinge width} = \text{IQR} = |\text{lower hinge}–\text{upper hinge}| \tag{1}$$

A lower inner fence (LIF) and an upper inner fence (UIF) are defined at 1½ × IQR away from the lower hinge towards the minimum value and the upper hinge toward the maximum, respectively. Algebraically, values (X) at the LIF and the UIF are estimated as:

$$X_{\text{LIF}} = X_{\text{LH}}–(1.5 \times \text{IQR}) \tag{2}$$

$$X_{\text{UIF}} = X_{\text{UH}} + (1.5 \times \text{IQR}) \tag{3}$$

The data values beyond the inner fences are considered as outliers. In this paper, the outliers corresponded with the geochemical anomalies, and the values beyond the upper hinge (X_{UIF}), rather than those of X_{LIF}, were taken into consideration only.

3.2. Singularity mapping technique

Formation of an ore deposit can be a complex, nonlinear process. The mineralisation process may occur repeatedly at different periods, and a deposit may be transformed many times by geological activities. The key conceptual issue supported by many studies is that the intensity, geometrical morphology and frequency distribution of anomalies related to mineralisation almost certainly will be different from anomalies that are related to a regional geological process (Cheng et al., 2007). Research on and application of nonlinear fractal theory and associated methods have proven that anomaly patterns, produced by different geological processes, have different scaling properties, anisotropy and general self-similarity characteristics (Cheng, 2007b). Thus, both anomaly and background information are present in geochemical sample data sets. Sampling may also be affected by other factors, such as sedimentation of aeolian sandy soil, landform, rainwash and vegetation. Because of these complex mechanisms, conventional statistical methods may be not effective in the treatment of geochemical data sets.

The local singularity index model was proposed by Cheng (1999), based on nonlinear fractal theory and was considered to be an effective method to characterise special phenomena accompanied by energy release or material accumulation within narrow spatial–temporal intervals. This singularity property has been observed in geochemical data sets (Ali et al., 2007; Cheng and Agterberg, 2009; Sun et al., 2010; Xiao et al., 2012; Zuo et al., 2009, 2013). This technique can advantageously be used to discriminate geochemical anomalies from regional or local backgrounds. For a two-dimensional situation, the principle of the singularity model can be quantitatively described by the following power–law relationships (Cheng, 2007a):

$$\mu(A_i) \propto A_i^{\frac{\alpha}{2}} \tag{4}$$

$$\rho(A_i) \propto A_i^{\frac{\alpha}{2}-1} \tag{5}$$

where $\mu(A_\text{i})$ and $\rho(A_\text{i})$ denote the amount and density of a certain physical quantity in an area (A_i), respectively. ∝ denotes proportionality and α is the estimated singularity index. When applied to a geochemical map, $\alpha > 2$ or $\alpha < 2$ represent enrichment and depletion of element concentrations, respectively (Cheng, 2007a; Zuo et al., 2013). At locations where the singularity index $\alpha \approx 2$, neither positive nor negative geochemical singularity is observed. Thus, singularities on a geochemical map can provide significant information for identifying geochemical anomalies associated with mineralisation (Xiao et al., 2012). More details associated with this method are available in other papers (Cheng, 2007a, 2011; Xiao et al., 2012; Zuo and Cheng, 2008; Zuo et al., 2013).

To estimate the local singularity from a geochemical map, in the present study, a window-based approach was used as follows:

Step 1 A spatial interpolation method was used to obtain raster maps from data sets, based on inverse distance weighted interpolation. All such raster maps were resampled with an appropriate spatial resolution (the spatial resolution is approximately 2 km), and four raster maps (Ag, As, Au and Sb) were produced in this step.

Step 2 Given a location on the map, a set of sliding windows $A(r_i)$ (square windows) with variable edge sizes, $r_i \times r_i$ ($r_i = 3, 5, 7, \ldots, 15 - r_i$ represent the number of cells along the edge of the sliding window) was used. For each window, the average concentration value $M_j[A(r_i)]$ ($j = 1, 2, 3, \ldots, n$) [n represents the total number of the grid in the raster map produced in Step 1] was calculated.

Step 3 The $M_j[A(r_i)]$ values for every location (j) show a linear trend with linear size r_i on log-log plot, or $\log M[A(r)] = c + (\alpha{-}2)\log(r)$. The points were fitted with a straight line by using the least squares method, and the slope of the linear relationship was assumed as the estimate of $(\alpha - 2)$, where α represented the singularity of location (j).

3.3. Principal component analysis

Principal component analysis (PCA) is a widely used multivariate statistical method in the treatment of geochemical data and mineral exploration studies (Cheng, 2008; Wang et al., 2012; Xiao et al., 2012; Zhao et al., 2012a; Zuo, 2011). Interrelated variables with high dimensionality can be transformed into several uncorrelated principal components (PCs) based on a covariance or correlation matrix using the PCA technique. A reduced number of PCs provides a more comprehensive and often more interpretable information for specific objectives.

4. Analysis of mono-element data distributions

A total of 1,444 stream sediment samples in the present data set were used in this study, which covered approximately 11,600 km^2. Silver, As, Au and Sb were selected. These analytical results of each element contained some extremes (Fig. 3). The frequency distributions of As (Fig. 3-B) and Au (Fig. 3-C) were clearly positively skewed distributions. While the frequency distributions of Ag (Fig. 3-A) and Sb (Fig. 3-D) tended to follow a normal distribution without consideration of the outliers. However, based on their quantile-quantile (Q-Q) plots, Ag, As, Au and Sb were not normally distributed (Fig. 4).

For more insight as to the distribution of single element, the data sets of Ag, As, Au and Sb were transformed by applying the natural logarithm method, and the frequency distribution plot (Fig. 5) and Q-Q plot (Fig. 6) were plotted. The four logarithmically transformed data sets appeared much more to follow a normal distribution. However, the Q-Q plot (Fig. 6) and the results of normality testing showed that the concentration data sets of the four elements still did not follow a normal distribution. Thus, the exploratory geochemical data set did not follow a log-normal distribution.

Two conventions were used in the ensuing data treatment:

1) A known gold deposit/occurrence is taken to be consistent with an anomaly if the distance of the deposit and the anomaly is shorter than 2 km (namely, the length of one grid on the raster map).

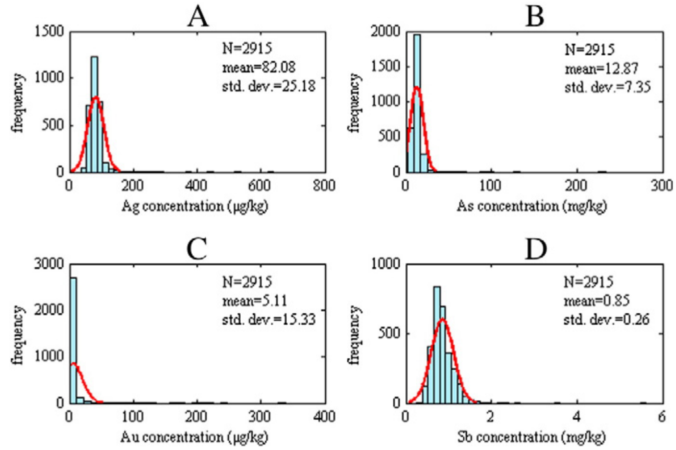

Fig. 3. Frequency distributions of Ag (A), As (B), Au (C) and Sb (D) concentration data from stream sediment samples.

2) The known gold deposits or gold occurrences are both called gold deposits, regardless of their size and scales.

5. Identification of geochemical anomalies using EDA

Interpolated geochemical raster maps were produced using the inverse distance weighting (IDW) for Ag, As, Au and Sb before the hard, global anomaly threshold was calculated by EDA. The maximum neighbours were 15 and minimum neighbours 10, and the cell size of these maps was approximately 2 km after resampling. The resulting thresholds for Ag, As, Au and Sb were 121.31 μg/kg, 20.55 mg/kg 6.71 μg/kg and 1.35 mg/kg respectively. The geochemical anomaly maps of Ag, As, Au and Sb are shown in Fig. 7-A to D.

The known gold deposits were closely related to the resulting Au anomalies (Fig. 7-C). The Au anomalies covered 12.11% of the study area, and 23 known gold deposits were consistent with Au anomalies, which accounted for 85.19% of the total known gold deposits. The known gold deposits are mainly located at the north and southwest districts of the study area, and the Au anomalies were also distributed over these two districts. The known gold deposits were not closely related to Ag, As and Sb anomalies (Fig. 7-A, B and D). The percentage of As, Cu and Zn anomalies in the study area were 2.92%, 5.39% and 3.26%, respectively, and only 33.3% (9), 40.74% (11) and 40.74% (11) known gold deposits were consistent with the Ag, As and Sb anomalies, respectively. The Ag, As and Sb anomalies were scattered over the study area and did not show a clear pattern.

6. Identification of geochemical anomalies using the singularity mapping technique

The singularity maps of Ag, As, Au and Sb were plotted (Fig. 8), and the singularity indexes were reclassified (natural breaks (Jenks) method was used) for quantitatively measuring the significance of spatial correlation between the areas with singularity < 2 and the locations of known gold deposits. The spatial distribution of Ag, As, Au and Sb anomalies relatively differed but showed that the known gold deposits were closely related to the lower singularity indices (and which are also less than two) of Ag, As, Au and Sb (Fig. 8). The lowest two classes of the singularity indices of Ag, As, Au and Sb (red and yellow coloured) accounted for 23.5%, 13.38%, 37.29% and 25.87% of the study area, respectively. In addition, 70.37% (19), 59.26% (16), 81.48% (22) and 66.67% (18) of known gold deposits were consistent with the anomalies of Ag, As, Au and Sb, respectively, which means that Ag, As, Au and Sb were appropriate indicator elements in the present study area, and the SM technique can identify gold deposit–related anomalies efficiently.

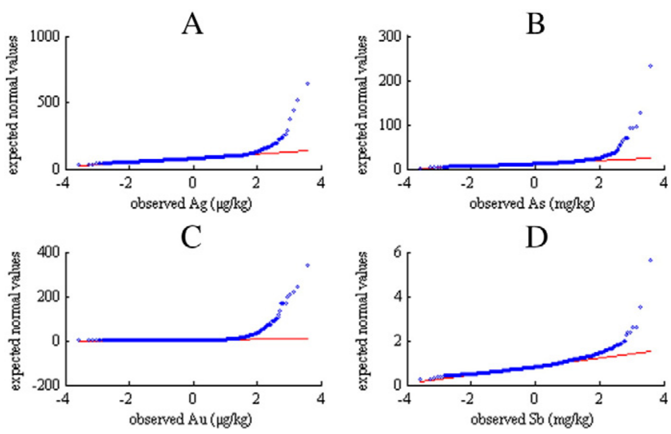

Fig. 4. Q-Q plots for the Ag (A), As (B), Au (C) and Sb (D) concentration data from stream sediment samples.

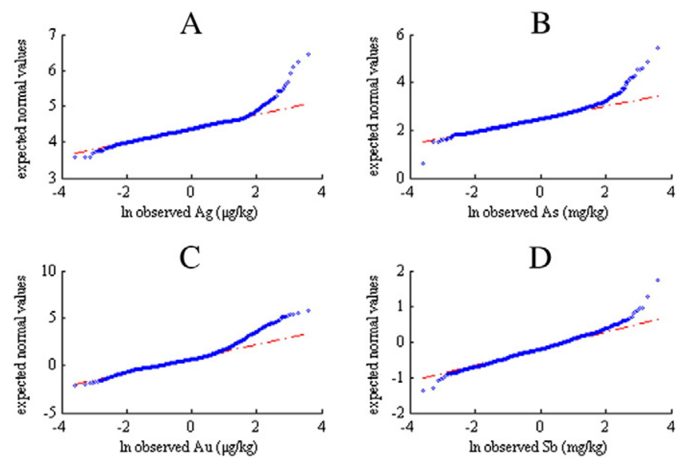

Fig. 6. Q-Q plots for the ln Ag (A), ln As (B), ln Au (C) and ln Sb (D) concentration data from stream sediment samples.

To reduce the uncertainty of a single element, and to obtain a more reliable results, PCA was used to delineate the comprehensive anomalous areas with the combined elements Ag, As, Au and Sb. Ordinary PCA uses a linear correlation matrix. A scree plot (Fig. 9a) shows the distribution of eigenvalues representing the relative importance of each component. The first principal component (PC1) accounted for 40.7% of the total variance while PC2, PC3 and PC4 modelled additional 23.1%, 21.0% and 15.2% of total variance, respectively. Positive loadings (Fig. 9b) indicated that PC1 mainly reflected the singular association of Ag, As, Au and Sb. Compared with the singularity maps of individual ore-forming elements, areas with the lower PC1 scores had stronger coincidence with known mineral occurrences (Fig. 10).

Furthermore, a noticeable spatial correlation exists between granite rocks, altered zones and fault traces with low PC1 scores, implying that these geological variables played an important role in the formation of known hydrothermal mineral deposits (Fig. 10; i.e., granite rocks may be the sources of energy and hydrothermal fluids, regional faults confine magmatic activities to certain scales and ranges, hydrothermal fluids permeate rocks through local faults, metasomatism and mineralisation occur within fault zones).

7. Results and discussion

Conventional statistical techniques that assume a data set follows normal or log-normal distribution may, therefore, not be suitable for geochemical data analysis, as the geochemical data sets in this study follow neither a normal nor a log-normal distributions, as shown in Section 3.

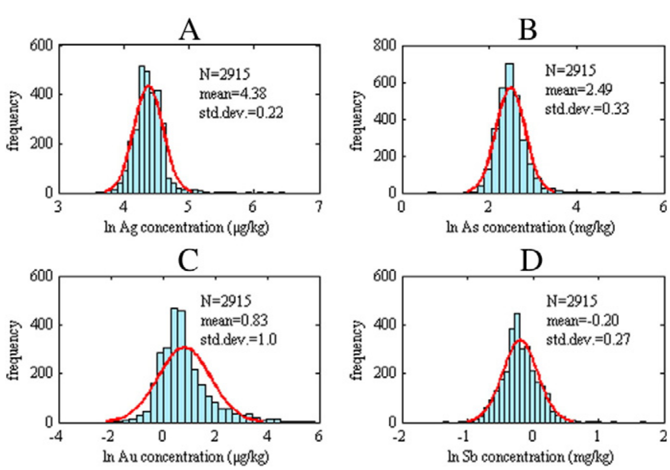

Fig. 5. Frequency distributions of ln Ag (A), ln As (B), ln Au (C) and ln Sb (D) concentration data from stream sediment samples.

Neither EDA nor the SM technique requires that the data set follows normal or log-normal distributions, and these two techniques were compared in detail in this study. The anomaly threshold definition is not seriously affected by outliers when EDA is applied, provided a robust approach is used, for example, MMDA. The EDA techniques have proven to be quite effective (Bounessah and Atkin, 2003) in the statistical treatment of single element stream sediment analytical results in areas where the data variability may be expected to be affected by lithological, sampling, analytical, climatic and physiographical factors. Using median and median absolute deviation instead of mean and the standard deviation, respectively, may be preferable when working with complex geochemical data (Templ et al., 2008). However, EDA is not suitable for identifying geochemical anomalies in the present study for the following reasons: (1) the present thresholds for Ag, As and Sb are all very high and only few anomalies exist on the corresponding map (Fig. 7-A, B, D). Although the known gold deposits are consistent with Au anomalies, the results may be unreliable because only few Au anomalies exist outside the areas of known gold deposits. Thus, the Au map provides only limited information for further mineral exploration; and (2) only one global threshold is obtained for each variable using EDA, which is not suitable for mineral exploration target prediction because this global level tends to overlook significantly weak anomalies, which mainly, or only, express themselves locally. These are effectively 'swamped' by a singular, high threshold levels. Such cases are obvious in study areas with complex geological backgrounds.

With the SM technique, singularity indices are used to identify anomalies. These indices will differ within the total spatial study area because of the sliding window approach. This has the effect that the SM technique does not overlook such local-scale weak anomalies, making it suitable for identifying geochemical anomalies. The results of this study show that PCA can be used to analyse the SM results of Ag, As, Au and Sb, and to obtain a more comprehensive and hopefully more meaningful end result. In this study, these results are exceedingly interpretable, when compared with the geological map of the study area. In some districts (Fig. 10; R1 and R2), the comprehensive geochemical anomalies are obvious, although no gold deposits have been found in those districts yet. R1 and R2 may thus be valuable potential districts for mineral exploration because telltale granite rocks, alteration zones and faults are indeed present.

8. Conclusions

1) The regional stream sediment geochemical data sets in this study neither follow a normal nor a log-normal distribution. EDA was not

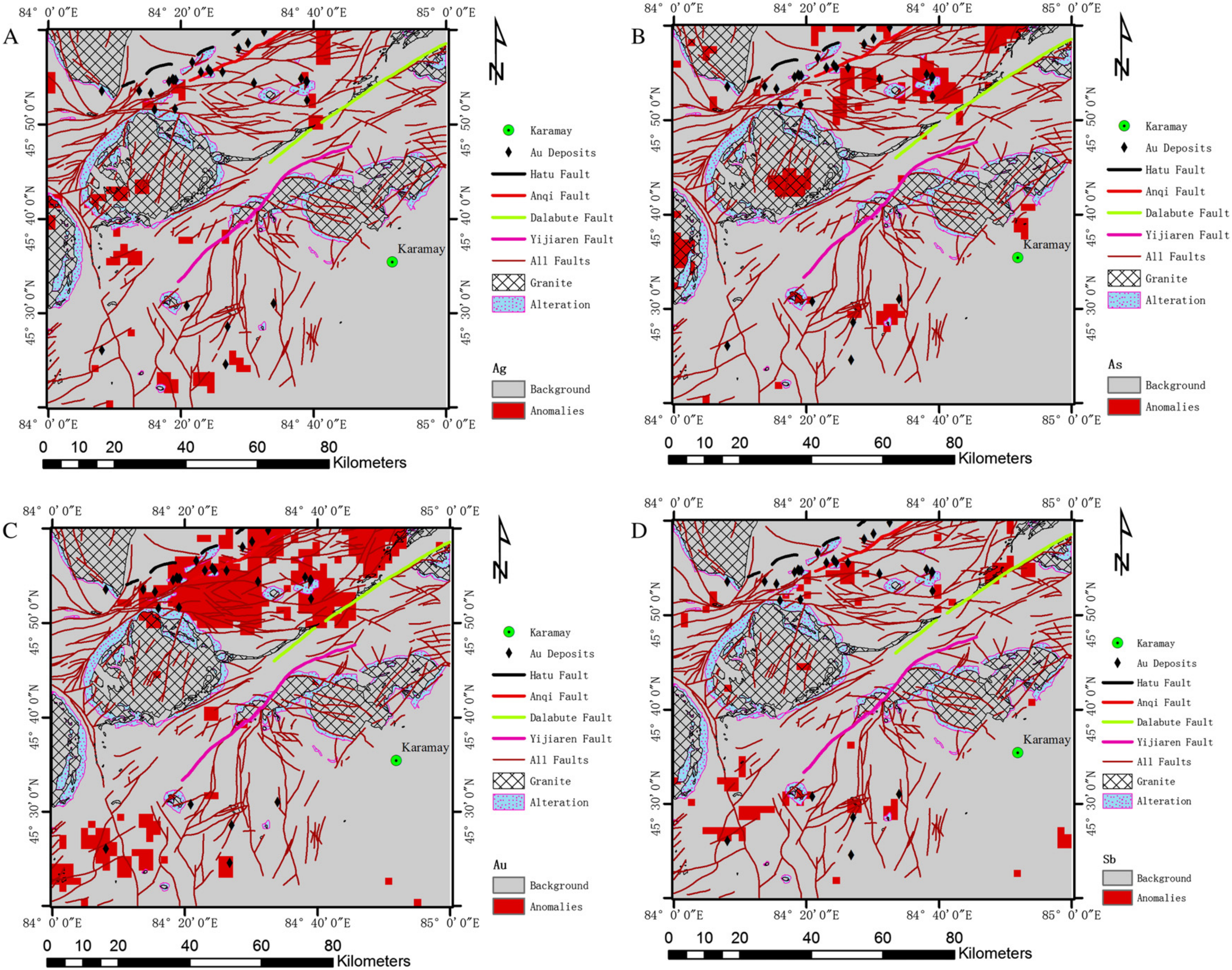

Fig. 7. Anomaly maps of Ag (A), As (B), Au (C) and Sb (D) generated from the EDA data treatment.

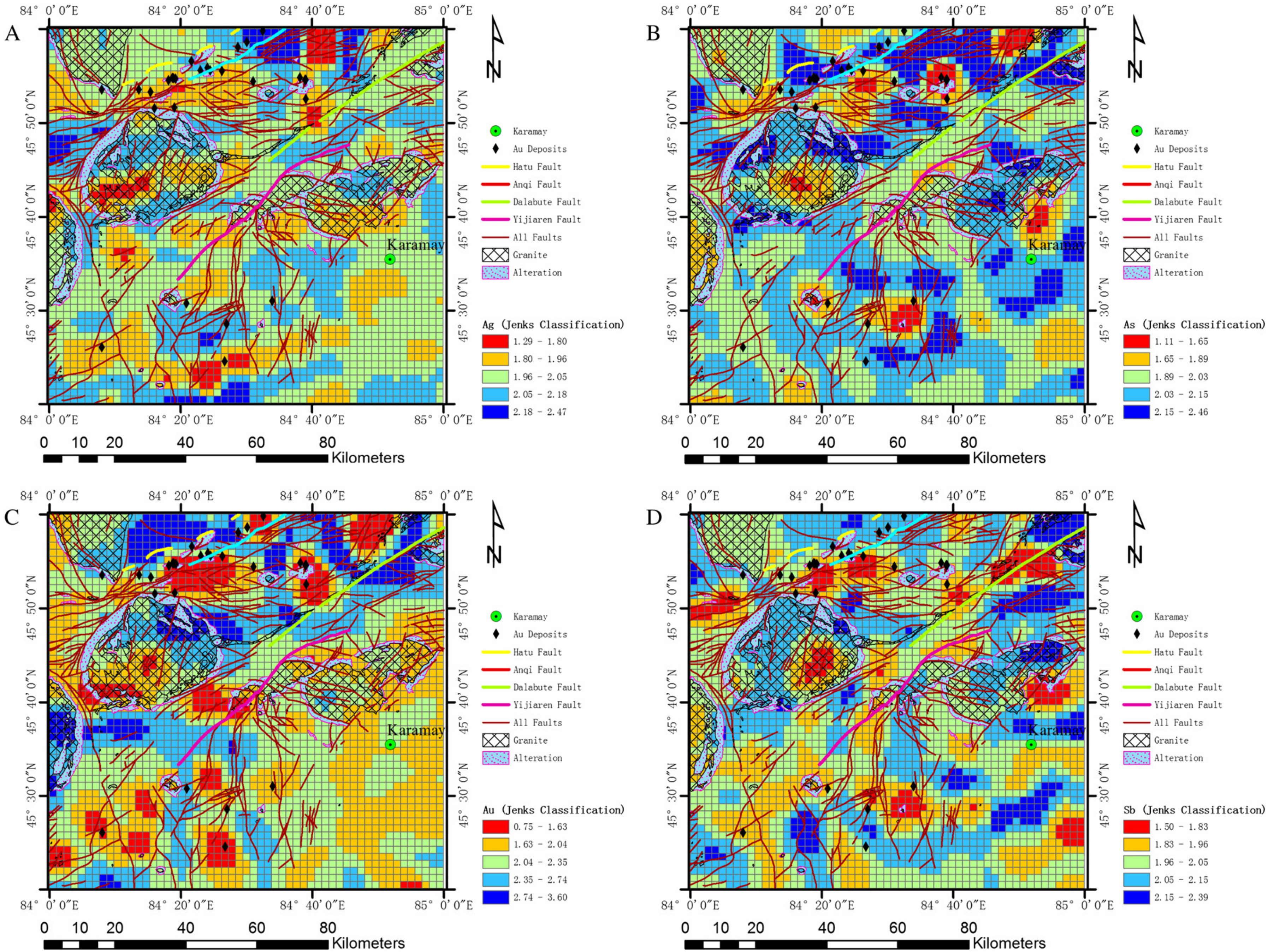

Fig. 8. Anomaly maps of Ag (A), As (B), Au (C) and Sb (D) generated by the singularity mapping technique.

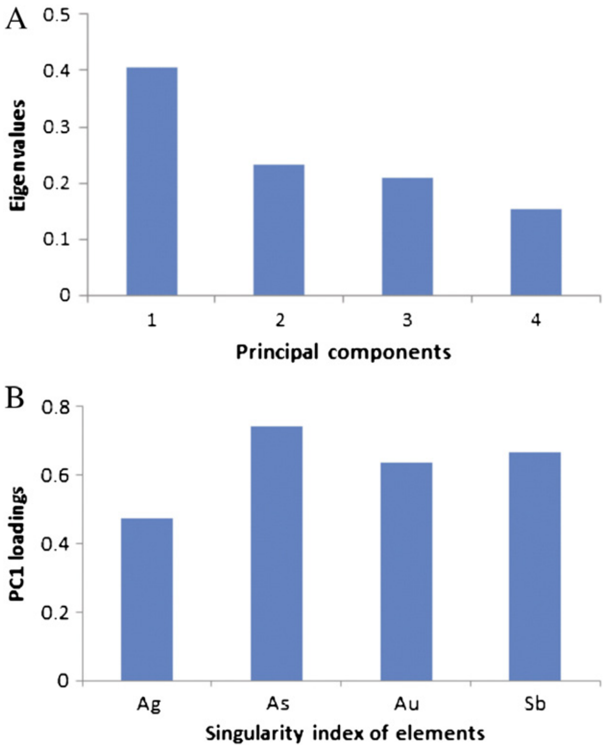

Fig. 9. PCA results on the geochemical data set. The geochemical data were processed using the local singularity analysis. Details are given in the text. (a) Scree plot of eigenvalues of principal components (PC1–PC4) of singularity indices of ore-forming elements; (b) loadings on the first component (PC1).

found suitable for identifying feasible anomalies in this study because it did not produce a clear, geologically interpretable geochemical anomaly pattern. By contrast, the SM technique was found exceptionally suitable for identifying geochemical anomalies, and when integrated with PCA, was shown to indeed be a powerful tool for identifying relevant anomalies in the Karamay geochemical data sets.

2) Silver, As, Au and Sb are appropriate indicator elements in the present study area, and in some parts (districts R1 and R2 in Fig. 10) where geochemical anomalies, rather than gold deposits are present, are identified using SM technique. They may be valuable for mineral exploration because of the merits of SM techniques, and geologically speaking, the identified comprehensive geochemical anomalies are explainable.

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Appendix A. Supplementary data

Supplementary data associated with this article can be found in the online version, at http://dx.doi.org/10.1016/j.gexplo.2014.12.007. These data include the Google map of the most important areas described in this article.

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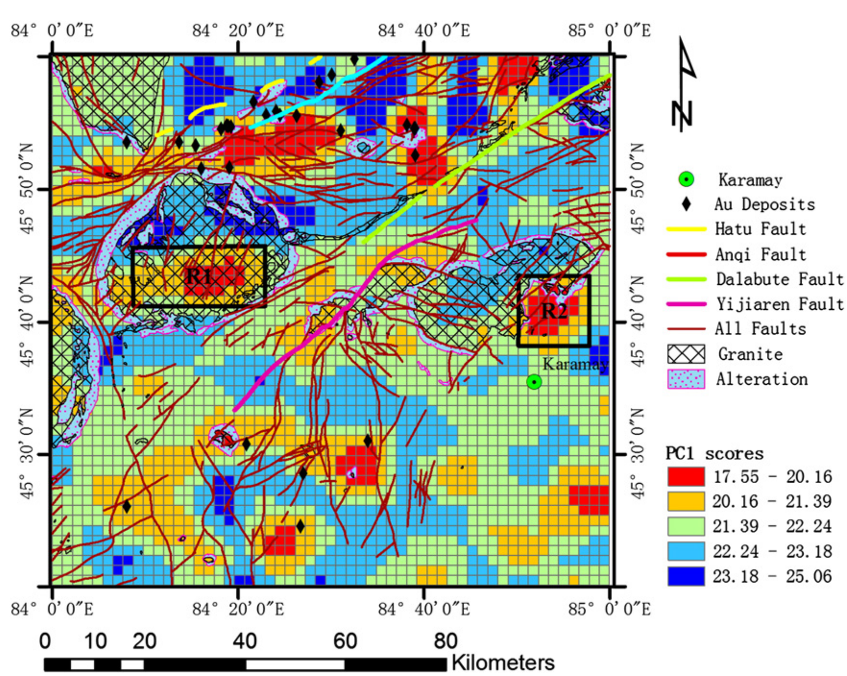

Fig. 10. Raster map showing the scores of samples on the first principal component (PC1).

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