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Analysis of geochemical patterns in a soil profile over mineralized bedrock

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Abstract
Transported soils cause difficulties in the identification of geochemical anomalies. It has been demonstrated that the joint application of Local Singularity Analysis (LSA) and Principal Component Analysis (PCA) can identify geochemical anomalies effectively, especially in regolith-covered areas. However, more convincing evidence is needed to explain the reasons for this. In this study, a soil profile overlying several mineralized veins cutting through the bedrock was analyzed in-situ using a portable X-ray fluorescence spectrometer. The patterns of two mineralization-related elements, Cu and Mo, were analyzed. The results revealed that the element concentrations of the soil sharply decreased as the distance from the bedrock increased, and this
relationship can be described by a power law model. The LSA enhanced several vein-like anomalies corresponding to the mineralization veins in the bedrock, and the presence of vertically elongated weak anomalies in the soil indicates the migration of ore elements originating from the underlying bedrock through the soil. The statistics show that the patterns of the Local Singularity Index (LSI) are stable at different depths and in different media, whereas the concentration patterns are not. In addition, the mineralization-related elements have a higher correlation coefficient for the LSI than for the concentration. Since a previous simulation study determined that a mineralization indicative first principal component prefers that the variables have a close relationship and that the variables have similar patterns in different geological objects, the patterns discovered in this study explain why LSA is effective in identifying geochemical anomalies, especially when combined with PCA.

**Keywords:** Regolith-dominated Area; Soil profile; Portable X-ray fluorescence spectrometer; Local singularity analysis; Data mining; Principal component analysis

Supplementary material: the high-resolution photo, the element concentration data and the lithologic data of the profile are available at GSL figshare portal.

1. **Introduction**

Mineral exploration in areas covered by regolith includes challenges, which require technological innovation in the mining industry (Gonzalez-Alvarez et al. 2016). The development of novel geochemical exploration techniques suitable for geochemical anomaly identification in areas covered by transported soils has attracted considerable attention from researchers. Many studies have demonstrated the mechanisms by which geochemical anomalies form, that is, elements can migrate...
from the underlying bedrock to the surface soils through electrochemical, biological, gaseous, and capillary processes (Hamilton 1998, Mann et al. 2005, Anand et al. 2014 2016). Laboratory experiments and field investigations have been conducted to trace element migration in soils (Mann et al. 2005). However, due to the limited number of case studies and the complexity of the lithology and regolith, the element migration patterns in soils are still unclear, which creates difficulty in anomaly identification and delineation in regolith-dominated areas.

As the development and utilization of modern data analysis techniques for mineral exploration, such as nonlinear methods and machine learning methods, evolve (Cheng 2007, Cheng 2012, Chen et al. 2014, Cheng 2014, Grunsky et al. 2014, Yang et al. 2015, Zuo, Wang et al. 2015, Chen 2016, Kirkwood et al. 2016, Zhao et al. 2016, Carranza 2017, Zuo et al. 2021, Parsa et al. 2021, Parsa, 2021, Parsa and Maghsoudi, 2021, Parsa and Carranza, 2021), complex patterns of geochemical element concentrations can be decomposed to enhance weak anomalies. In particular, in recent years, many improvements have been made to Local Singularity Analysis (LSA), including anisotropy (Wang et al. 2018), non-uniformity (Zhang et al. 2016), self-adaption (Xiao et al. 2016), and robust statistics (Zuo, 2014) have been proposed. This may allow the more effective utilization of geochemical data for different scenes. In particular, it has been demonstrated that the joint application of LSA and Principal Component Analysis (PCA) can efficiently identify geochemical anomalies, especially in regolith-covered areas (Cheng 2007, Cheng and Agterberg 2009, Zhao et al. 2012, Wang et al. 2015, Zuo et al. 2015).

Cheng (2012) mathematically proved that the Local Singularity Index (LSI) of a geochemical anomaly does not change with distance from the main reservoir to the surface, whereas the element concentration sharply decreases. A further simulation conducted by Zuo et al. (2016) revealed that
the LSI can indicate buried mineral deposits. Therefore, the LSI can be used as a generic index for quantifying the enrichment of an anomaly. In practice, LSA has been demonstrated to have the capacity for identifying geochemical anomalies in regolith-dominated areas (Cheng 2012). However, more evidence should be obtained to support the theory that the singularity of a geochemical anomaly is less influenced by the regolith layer.

As a commonly used multivariable analysis method, PCA and its derivative methods, such as robust PCA (Filzmoser, 1999), spatially weighted PCA (Cheng et al., 2011), and kernel PCA (Liu et al., 2016), have been proven to be universal in geochemical data processing. PCA can be used to construct Principle Components (PCs), which are linear combinations of elements that reflect the causal relationships with geological processes (Grunsky 2010). In addition, when the number of variables for a random process exceeds the required dimension for modeling the signal, the first few PCs have a higher signal-to-noise ratio (Vaseghi 2008). Therefore, PCA can integrate several mineralization associated element maps into a PC1 score map, which can indicate the presence of mineralization more efficiently. The Monte-Carlo simulation research conducted by Yang et al. (2019a) demonstrated that to acquire a stable PC1 score map, which can effectively indicate mineralization, one should: 1) use variables for which the geological objects have small differences, and 2) use variables with strong relationships. The successful joint applications of LSA and PCA in regolith-covered areas indicated that LSA must enhance PCA. However, more evidence should be obtained to explain this phenomenon, and more investigations of geochemical patterns in regolith layers may provide clues. In recent years, portable X-ray fluorescence spectrometry (pXRF) has been successfully used in high spatial resolution qualitative and quantitative studies of geological processes (Yuan et al. 2020, 2021). Hence, it is possible to use pXRF to collect element data for
regolith layers in field investigations, and the patterns of these data may help us to understand how LSA and PCA coordinate. In this study, a soil profile cutting across regolith layers and altered bedrock containing mineralized veins was analyzed in-situ using pXRF. PCA and LSA were applied to reveal the patterns of the elements in the profile in order to determine the reason that LSA is efficient in regolith-covered areas, especially when combined with PCA.

2. Methodology

2.1 Local Singularity Analysis

Local singularity analysis is a spatial data processing technique developed in the context of multifractal theory, which can characterize the complex and anomalous patterns of geochemical element concentrations (Cheng 2007). In the mathematical formula for LSA, the average concentration $\rho(A)$ of a chemical element in a small area $A$ of a linear size $\varepsilon$ satisfies

$$<\rho(A)> = c\varepsilon^{-\Delta\alpha}, \quad [1]$$

where $<*>$ denotes the expectation of $*$, $\Delta\alpha$ is the local singularity index, and $c$ is the fractal density. When the scale $\varepsilon$ approaches zero, the above power-law usually exists in a statistical sense. The values of $c$ and $\Delta\alpha$ are independent of $\varepsilon$. Additionally, when the element distribution is isotropic, these two parameters are independent of the scale $A$. The values of both $c$ and $\Delta\alpha$ vary with location. The local singularity index $\Delta\alpha$ can be estimated using different methods, and many algorithms considering sophisticated geological situations have been developed in recent years, such as the fault-oriented local singularity index (Wang et al. 2013), the anisotropic singularity (Wang et al. 2018), and the LSI with removal of local minima (Zuo et al. 2015). The classical and most commonly used method is the window-based method developed by Cheng and Agterberg (2009), in
which for a given location on a geochemical map, a series of windows with sizes of \( 0 < r_1 < \cdots < r_n \) can be defined accordingly, and the average concentration in each window \( \rho(r_i) \) can be calculated from the total sum of the values of the samples located within the window. These average values, \( \rho(r_i) \), can be plotted against \( r_i \) on a log-log plot, and the linear trend of the plot can be fitted using the least squares method, which provides an estimate of the slope \( -\Delta \alpha \) and intercept \( \log c \). In this study, the classical one-dimensional LSA was used to process the concentration data for the soil profile.

### 2.2 Principal Component Analysis

Principal component analysis uses an orthogonal transformation to convert a set of observations into a sequence of linearly uncorrelated principal components. The steps of the implementation of classical PCA have been described in many papers (e.g., Yang and Cheng 2015, Parsa et al., 2017). In order to interpret the meaning of the components obtained via PCA, prior knowledge of the input data and the background geology of the sampled area is required (Grunsky 2010, Carranza 2011, Wang et al. 2011, De Caritat et al. 2016, Grunsky et al. 2017). In this situation, the interpretation of the components is based on the compositions of the first few PCs, which represent interpretable predominant processes, while the minor PCs represent noise or under-sampled processes (Grunsky et al. 2014). When the number of variables for a random process exceeds the required dimension for the modeling of a process, the first few components may more efficiently indicate the process (Vaseghi 2008). Therefore, if a mineralization process can be represented by several strongly associated mineralization-related elements, a PC1 score map of these elements may indicate the presence of deposits more efficiently. The Monte-Carlo simulation conducted by Yang et al. (2019a) proved that
a mineralization indicative PC1 prefers that the variables of the geological objects have small differences and the variables have strong relationships. Therefore, the differences among the geological objects and the relationships between the variables should be measured. The relationships between the variables can be reflected by the Pearson correlation coefficient. The differences among geological objects can be divided into two aspects: the differences in the relationships between the variables and the differences in the mean values of the variables. These two aspects can be depicted using a combination of PCA and a scatter plot. The PCs of a population can roughly delineate the relationships between the variables. The difference between two populations can be roughly denoted as the angles between PC1s, and its cosine value can be quantified as the dot product between the PC1s. The differences in the mean values of the variables can represent the distance between two populations’ centers, which can be shown as the intersections of the PCs. In the following analysis, the similarity between geological objects and the relationship between elements are investigated using scatter plots and PCA.

3. Geology and geochemical data

The soil profile in this study is an outcrop section of a profile cutting across altered rock containing mineralized veins in the Dalaimiao district, Inner Mongolia, China. The Dalaimiao district is a typical arid grassland with smooth topography. Due to intensive aeolian processes, about 60% of the district is covered by a thin layer of wind-transported sand and silt, and over 40% of the area is mapped as Cenozoic regolith (Yang et al. 2019b). Over the Wulandele Mo-Cu hydrothermal deposit, which is located in the Dalaimiao district, several exploratory trenches were dug, exposing a fresh section that contained both mineralization veins and the soil layers for this study. This section measured 63 cm × 50 cm (width × height) and was divided into the A, B, C, and R horizons (Fig. 1a).
The A horizon was brown in color and consisted of wind transformed till, sand, a few plant roots, and some rock debris from nearby outcrops. In contrast to the A horizon, the B horizon was a darker color, lacked organic material, and was enriched in iron. The C horizon consisted of large blocks of whitish weathered bedrock composed of carbonate and gypsum. The R horizon was composed of fresh quartz diorite. Three sericite quartz veins with Mo-Cu mineralization intruded the C horizon and R horizon almost vertically (Fig. 1-b).

The profile was analyzed using a portable X-ray fluorescence spectrometer (Niton XL3t 950), which was equipped with a silicon drift detector with an energy resolution of better than 185 eV, a 50 kV and 40 µA X-ray tube, and an 8 mm diameter test window. The stability and accuracy of the equipment had previously been tested using different samples, including liquid, biological, and silicious samples during the last few years (Zhou et al. 2018, 2020a, 2020b). Moreover, because the following quantitative analysis is based on log-transformed or local singularity analyzed data, the prior calibration of the elements, which was based on a linear transform, was not essential. There were 326 analysis spots in the profile, and each was analyzed for 65 seconds. In the horizontal direction, the sampling interval between two adjacent spots was 2 cm in the A and B horizons and 3–5 cm in the C and R horizons. The locations of the sampling spots are shown in Figure 1b. Cu and Mo were chosen for analysis because the main mineralization was molybdenite and chalcopyrite, and most of the concentration values of these two elements were higher than the detection limits of the pXRF. Then, the raw data were interpolated using the ordinary Kriging method using an exponential model and a grid cell size of 1 cm × 1 cm (Fig. 2). The Mo (Fig. 2-a) and Cu (Fig. 2-b) concentration maps show that high concentration values commonly coincided with the locations of the quartz veins in the diorite. The Cu and Mo concentrations of the bedrock (C and R horizons) were much higher.
than those of the overlying soils (A and B horizons). The changes in their concentrations clearly delineated the boundary between the bedrock and the soils. The Cu and Mo concentrations of the bedrock were not only high but also exhibited vertical elongated anomalies that spatially coincided with the quartz veins. However, the concentrations of the soils did not exhibit any significant trends.

4. Analysis of the geochemical patterns

4.1 Relationship between element concentration and distance to bedrock

To quantify the decay trend of the Cu and Mo concentrations along the vertical profile, the geometric means of the concentration values that were located the same distance from the weathered bedrock (C horizon) were calculated. The values were plotted against the distances between the sample locations and the bedrock surface (Fig. 3). As shown in Figure 3, the mean values decreased as the distance between the sample location and bedrock increased, exhibiting a power law or linear relationship on the log-log plots. This pattern verifies that the element migration processes follow a fractal law, which has also been demonstrated by Cheng (2012, 2014). Moreover, the coefficients of determination of the least squares fitting between the log-transformed concentration and log-transformed distance are $R^2 = 0.684$ for Cu and $R^2 = 0.375$ for Mo. The slopes of the linear regressions are $-0.367$ for Cu and $-0.158$ for Mo. The difference between the slopes estimated for Cu and Mo ($0.367 > 0.158$) demonstrates that the Cu concentration decreased more dramatically than the Mo concentration, which led to changes in the elements’ relationship at different depths in the soil.

4.2 Element concentration patterns

To further investigate the relationship between Cu and Mo at different sampling depths, datasets
at depths of 0 cm, 5 cm, 10 cm, 30 cm, 35 cm, and 40 cm were extracted from both the concentration and LSI maps. The first three sampling depths were in the soil (A and B horizons) and the other three were in the fresh bedrock (R horizon). The names of the datasets were labeled to denote the depth and source. For example, the dataset obtained from the concentration map at a depth of 0 cm is labeled C0, and the LSI dataset at a depth of 5 cm is labeled S5.

Considering the positive skewness, the concentrations were log-transformed using a log base of 2 and were plotted in Figure 4. Two significant groups (populations) can be observed in Figure 4a, and each group contains three datasets from soil or bedrock. Through comparison of these three soil datasets, it was found that their centers (intersections of PC1 and PC2) are dispersed, and the dataset collected at a deeper depth is closer to the original point, indicating that the concentrations of the soil decrease with increasing distance from the bedrock. However, the centers of the datasets from the bedrock tend to be close to each other, and no obvious change occurs with increasing sampling depth. The similarity of the relationship between the elements can be characterized by the PCs. The three PC1s obtained from the same medium have similar directions, whereas the PC1s obtained from different media have significantly different directions. To quantify the similarity between the PC1s, the dot products of the PC1s are presented in the Table 1 (larger values represent a more similar element relationship, the maximum value is 1, and the minimum value is 0). Table 1 shows that for the values in the first three groups or the last three groups within the same sampling medium, the correlation between the two PC1s is close to 1; and for two datasets from different media, the correlation is close to 0. This implies that the relationship between Cu and Mo is similar within the same medium but is significantly different in different media. In addition, from C0 to C5 to C10, the similarity decreases (e.g., the dot product for C0 and C5 is 0.997, and the dot product for C0 and C10
is 0.945), which implies that the divergences of the concentration data from different depths increases with increasing sampling depth.

The clear divergences of the patterns for the different media and different sampling depths also can be observed in the boxplot of those six datasets (Fig. 5). Figure 5-a shows that the quantile statistics of the soil Cu concentration dataset significantly increase with increasing depth, but the quantile statistics of the bedrock datasets are approximately stable and are generally higher than the statistics of the soil datasets. Similar patterns also occur for the Mo concentration datasets (Fig. 5-b). The correlation coefficient between the log-transformed Cu and Mo concentrations was calculated, and the results are shown as the red line in Figure 6. The correlation coefficient is about 0.5 for the datasets from different depths. It is obvious that when the sampling depth is close to the interface between the soil and bedrock, the correlation coefficient between Cu and Mo decreases. This may be because the material’s composition changes near the interface, and this causes a change in the relationship between these elements.

4.3 Patterns of the local singularity index

One-dimensional LSA was performed in the horizontal direction to create two LSI maps (Fig. 7a and b). The maps indicate that the high LSI values have a high spatial coincidence with the mineralized quartz veins in the bedrock. According to the research conducted by Yousefi (2017), a multiplication process on data could contribute to better visualization of the mineralization; therefore, the fractal dimension values of Mo and Cu (fractal dimension value equaled the LSI value plus one in this case, because one dimensional LSA was performed) were multiplied and are shown in Figure 7c. Because PCA can also enhance anomalies when the input variables are highly
associated with the mineralization, PCA was applied to the LSI maps, and the PC1 map is shown in Figure 7d. It can be seen that these two data processing steps resulted in similar results, and on both maps, the anomalies have a stronger spatial association with the mineralized quartz veins. Moreover, several vertically elongated weak anomalies in the soil originate from the mineralized quartz veins, and these anomalies reach the surface. This may indicate the migration of the ore elements originating from the underlying bedrock through the soil. Moreover, from the bedrock to the surface of the soils, these LSI anomalies do not exhibit obvious decreasing trends.

Unlike the concentration patterns in Figure 4a, the six LSI datasets are almost mixed into one population (Fig. 4b), indicating that the LSI values for Cu and Mo in all six subgroups are similar. This pattern can also be observed in the boxplots showing the LSI datasets for Cu and Mo (Fig. 5c and d). Although the datasets for the different media have differences in the first and third quartile, no obvious difference was found in the median or average values. In addition, the statistics of the soil datasets do not exhibit obvious decreasing trends. This implies that the intensity of the LSI in the regolith is not or less affected by the distance to the bedrock. With respect to the correlation between the variables, the correlation coefficient between Cu and Mo is shown as the blue line in Figure 6. It can be seen that the correlation coefficient of the LSI is approximately 0.7. This value is larger than the value for the concentration (0.5), which implies that the mineralization-related elements have a closer relationship with the LSI. In addition, the curve of the LSI is flatter than the curve of the concentration, which implies that the elements have a more stable relationship at different depths and in different media.

With respect to the similarity of the relationship between the elements, Figure 4b also shows that the PC1s of the singularity datasets have more similar directions than the PC1s of the concentration
datasets for the same medium. The dot products of the PC1s of the singularity datasets are presented in Table 2. Through comparison of Table 1 and Table 2, it was also found that the dot products of the PC1s of the element LSI values are generally greater than those for the concentrations. This implies that: 1) the elements in the singularity have a more similar correlation relationship in the different media, and 2) the sampling depth almost does not significantly alter the correlation between the elements.

5. Discussion and Conclusions

The results obtained by analyzing the distributions of the Cu and Mo in a soil profile above mineralized bedrock revealed that the element concentrations of the soil sharply decrease with increasing distance from the bedrock, and the correlation coefficients between the elements vary at different sampling depths and in different media. The decreasing trend of the Cu and Mo concentrations with increasing distance between the samples and bedrock can be described by a power law (fractal) model. The power law relationship between the concentration and the distance to the bedrock is similar to that reported for soils more than 20 m thick (Cheng 2014). The phenomenon that the element concentrations of the soil sharply decrease with increasing distance from the mineralization explains why it is difficult to detect element concentration anomalies on the surface. Moreover, because the thickness of the soil or regolith is usually unknown, the same concentration measured at the surface may represent different intensities of the mineralization in the bedrock.

However, the LSI not only highlighted the weak Cu and Mo anomalies in the soils, which were similar to those in the bedrock but it also revealed the similar relationships between Cu and Mo in both the soils and bedrock. These facts suggest a generic link between the weak anomalies in the
soils and in the underlying bedrock. In addition, this phenomenon validates the conclusion of the mathematical proof and the numerical simulations; that is, the LSI is relatively independent of the distance between the sampling location and the bedrock. This property makes LSA a useful method for identifying weak anomalies, especially those caused by buried mineralization in regolith-dominated areas. It must be emphasized again that the simulations conducted by Yang et. al (2019) proved that a mineralization indicative PC1 prefers the variables in which the geological objects have small differences and close relationships. In this study, the mean values and the relationship between the elements in the singularity index were stable at different depths and in different media. Moreover, after the LSA, the mineralization-related elements had a closer relationship (a higher correlation coefficient). These two facts explain why the joint application of PCA and LSA effectively identifies geochemical anomalies.

Acknowledgements

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Reference


Figure 1. Horizons and geological map of the soil profile. (a) A Photo of the soil profile. The soil profile can be classified into four horizons: the A horizon is brown (rich in organics), the B horizon is brown-black (rich in iron), the C horizon is white (rich in calcium), and the R horizon is fresh bedrock. (b) Geological map of the soil profile. Three parallel mineralization quartz veins cut across the bedrock and the C horizon. The black dots are the in-situ analysis locations.
Figure 2. Element concentration maps for Mo and Cu showing the elements’ distributions in the soil profile. (a) Mo concentration map. In the C and R horizons, the high concentration values coincide with the three mineralization veins, and in the soil layer (A and B horizons), the concentration gradually decreases from the bottom to the top. (b) Cu concentration map. The patterns of (b) are rather similar to those in (a), but the high concentration values coincide with the mineralization veins on the two sides.
Figure 3. Log-log plot showing the relationship between the geometrical means of the concentration values and the sampling locations. A power-law relationship can be used to model the relationship between the concentration value and the distance to the bedrock. The bases used for the log transform was 2 for concentration and was 10 for distance.

\[ y = -0.1577x + 1.1341 \]
\[ R^2 = 0.3749 \]

\[ y = -0.3672x + 2.0534 \]
\[ R^2 = 0.6844 \]
Figure 4. PCA scatter plots of the element data for different depths. (a) Mo vs. Cu (log-transformed concentration); and (b) Mo vs. Cu (local singularity index). The datasets for different depths are labeled with different colors. Every dataset has two crossed arrows; the longer one is PC1, and the shorter one is PC2, and the intersection of the two arrows represents the center (mean) of the dataset.
Figure 5. Boxplot showing the datasets for different depths. The red square in the box denotes the average, the red line in the box represents the median, the upper and lower boundaries of the box are Q3 and Q1, respectively, the upper whisker is Q3 + 1.5*IQR, and the lower whisker is Q1 – 1.5*IQR, where IQR is the interquartile range (Q3-Q1). (a) Datasets for log-transformed Cu concentration; (b) Datasets of log-transformed Mo concentration; (c) Datasets for Cu local singularity index; and (d) Datasets for Mo local singularity index.
Figure 6. Plot of the correlation coefficient between Cu and Mo versus sampling depth. The blue line is for the local singularity index, and the red line is for the log-transformed concentration.
Figure 7. Local singularity index maps of the soil profile. (a) Mo, (b) Cu, (c) Dimension product of Cu and Mo, and (d) PC1 of the LSI of Cu and Mo.
Table 1. Dot products of the PC1s of the element log-transformed concentration datasets

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Table 2. Dot products of the PC1s of the element local singularity index datasets

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