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Research Paper

Identification and Separation of Geochemical Halos Using Hierarchical Clustering, Singularity, and Support Vector Machine Methods

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Abstract: In exploratory projects, the identification of geochemical anomalies in different areas may become complicated under the influence of geological processes. To solve these ambiguities, different methods should be used for a correct understanding of the available information. In this research, by expressing the concept of hierarchical clustering to identify elements related to mineralization, singularity, and how to draw singularity maps in the form of multifractal models and support vector machine method, the anomalous areas where there is a possibility of mineralization are seprated from the context regions. At first, two elements, gold and copper, were identified as elements related to mineralization in the created clusters using the hierarchical clustering method and Ward's method. To calculate the singularity index of these two elements, the method based on the window and the power relation of grade area was used at each point. Finally, by separating the singularity index values into two parts, training and testing, and with the help of the SVM method, the process of classification and estimation of singularity index values was done to identify anomalous areas for unknown areas. A case study has been carried out on the data of the porphyry copper deposit rich in Dali gold with an area of 900×800 meters located in the Urmia-Dokhtar magmatic belt. The data is related to surface soil samples in the target area. The results of this method are consistent with the previous studies conducted in the region. The results of the hybrid method used in this research show good agreement with previous studies. As a result, the use of these introduced hybrid methods can be a suitable guide for the production of geochemical maps in unknown areas.

Keywords: Hierarchical clustering, Singularity, Support vector machine, Porphyry copper.

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INTRODUCTION

One of the important processes in exploration data analysis is the identification of geochemical anomalies to determine promising areas for mineralization. In these studies, statistical and mathematical methods (non-structural methods) are used to separate anomalies from each other. These methods include element concentration frequency histogram analysis and univariate or multivariate statistical analysis [1]. These methods have limitations such as the condition of following the normal distribution, removing some data as out of line, not paying attention to the spatial distribution of the data, not paying attention to the geometric shape of the anomalies, and also the difficulties of working with large data [2]. Therefore, to solve these limitations, studies are focused on the use of classification methods to identify the relationship between the elements related to mineralization and the separation of anomalies [3]. One of the major advantages of fractal models compared to the statistical methods used in the separation of geochemical anomalies is the consideration of the spatial location of the samples. Classification methods are the most important part of the exploratory data modeling method. For this purpose, several machine learning methods have been developed in recent decades, such as artificial neural networks, support vector machines, and random forests [4]. In this research, using the hierarchical clustering method and placing elements in the created clusters, the elements related to specific mineralization and other elements were removed from the modeling process. By examining the singularity index and classifying the results with the support vector machine method, anomalous areas were identified in the exploratory area of Dali.

METHODS

Based on exploratory studies carried out in the Dali region located in the Urmia-Dokhtar volcanic belt, gold-rich porphyry copper mineralization has been evaluated. The studied region has an area of 900×800 meters, in which 149 topsoil samples were taken scattered under a 50×50-meter square grid.

Hierarchical Clustering

In the hierarchical clustering method, the connection algorithm is used in such a way that the variables or samples with more similarity are connected using the aggregate method (connection from the bottom to the top) or divisional method (connection from the top to the bottom) [5]. One of the important applications of the hierarchical clustering method as a data-oriented approach is to determine the relationship of geochemical elements related to mineralization. According to the identification of the element related to mineralization, further analysis can be done on these known elements [3].

Singularity

Mineralization processes can be modeled as fractal or multi-fractal, depending on the order of enrichment and dispersion of the concentration of geochemical elements. The singularity index is used to determine the geochemical complexity related to the mineralization process in a multi-fractal field. This method is useful in separating geochemical and geophysical anomalies from the background value. In general, the principle of the singularity model is defined by power relations 1 and 2 [4]:

$$\mu(A) \propto A^{(\alpha/2)} \Rightarrow \mu(A) = kA^{(\alpha/2)} \quad (1)$$

$$C(A) \propto A^{(\alpha/2-1)} \Rightarrow C(A) = kA^{(\alpha/2-1)} \quad (2)$$

Where:

A: is the area,

μ(A): is the total amount of metal in the area A,

C(A): is the average concentration in the area A,

k: is the numerical constant,

α: is the singularity index.

In the condition that the singularity index is positive ($\alpha>2$), the calculated average concentration decreases with the decrease of the size of A, which shows the areas with background values. In the negative singularity index ($\alpha<2$), the calculated average concentration increases with the decrease of the size of A, which indicates anomalous areas. As a result, calculating the values of the singularity index and preparing the singularity map can create suitable spatial patterns for the exploration of unknown areas [6].

Support Vector Machine

A support vector machine is a binary classifier that separates two classes using a linear boundary and is related to the family of generalized linear classifications. This algorithm finds a hyperplane that can act in a way that while being compatible with the training data, can separate the data sets from each other [7]. The application of this method in mineral potential mapping [8] and identification of alterations containing mineralization has also been proven [9].

FINDINGS AND ARGUMENT

In this research, using Ward's method, the Euclidean distance similarity matrix has been used for connection according to relation 3.

$$\boldsymbol{d_{AB}} = \sqrt{\sum_{i=1}^{m}(\boldsymbol{X_{iA}} - \boldsymbol{X_{iB}})^2} \quad (3)$$

Where:

$\boldsymbol{d_{AB}}$: is the distance of sample A from B

$\boldsymbol{m}$: is the number of variables.

According to the tree diagram resulting from the hierarchical clustering for the regional data, the elements are grouped into clusters. Based on this, the two elements of gold and copper are placed in one cluster which indicates the relationship of these two elements with each other, which is related to the mineralization of gold-rich porphyry copper type. According to the results of hierarchical clustering and the concentration distribution of copper and gold elements in the desired range for calculating α values, several points are considered. At the center of each point, there are five square areas with dimensions of 60×60 m, 120×120 m, 180×180 m, 240×240 m, and 300×300 m which are created in the GIS environment. To model using the support vector machine method, the singularity index values for the two elements of gold and coppercalculated in the previous step for the region, have been divided into two parts of training and testing data. LibSVM function and RBF kernel function have been used to model and to estimate singularity values in other areas of the region. The Grid search method with a 5-fold validation method has been used to determine the optimal values of model parameters (c and γ). The optimal values of c and γ for the two elements of gold and copper are presented in Table 1. Then, the classifier model was created on the training data and evaluated by the test data. The results of the model evaluation can be seen in Table 2.

Table 1. Optimal parameters calculated by the Grid search method

Element	c	γ
Au	16	1.73E-04
Cu	2	1.03E-04

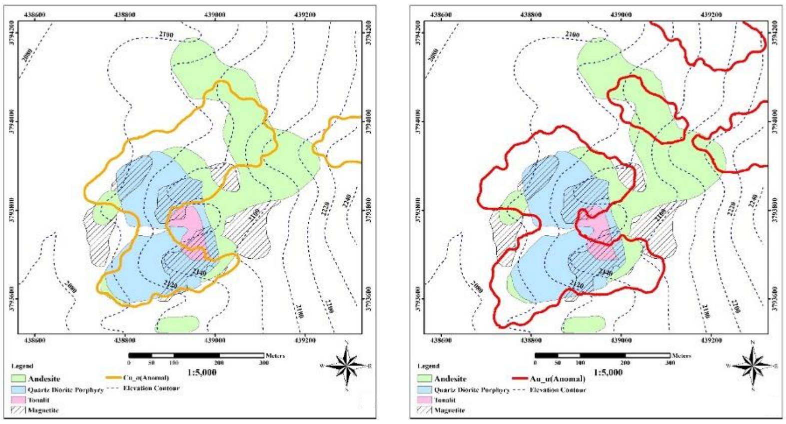
Table 2. Model evaluation parameters according to the test data

Accuracy of the model	RSME
80.65%	0.44

To predict the singularity index in unknown areas, the desirability of the evaluation results of the models was considered. The obtained results were drawn in the form of a singularity index map for two elements of gold and copper. Then, according to the magnetic anomalies identified in the region, as well as existing geological maps and the average concentration of Cu and Au in the soil, which are 0.1-0.5% and 0.3-2.9 g/t, respectively, the singularity distribution map was prepared using the SVM method, which shows a good overlap between the anomalous areas resulting from the estimation by the SVM method and the magnetic anomalies recorded in the area (Figure 1A and 1B).

CONCLUSIONS

In the singularity method, which is expressed in the form of fractal and multifractal models, the spatial position of each sample is considered by presenting singularity maps. As a result, it can distinguish anomalous communities from background values and detect pseudo and hidden anomalies more accurately.



(A) **(B)**

Figure 1. Singularity distribution map (α>2) estimated by SVM method for Cu and Au elements. **A:** Overlap of gold singularity and porphyry quartz diorite rock, andesite and magnetic anomaly range; **B:** Overlap of copper singularity and porphyry quartz diorite rock, andesite and magnetic anomaly range

The SVM method, which is considered as one of the machine learning methods, is a useful tool for identifying geochemical anomalies by classifying and estimating singularity index values. Finally, it can be stated that the use of these combined methods can be a good guide for producing geochemical maps in unknown areas. In this research, the grid search method has been used to determine the parameters of the support vector machine model. It is suggested to investigate the use of meta-heuristic optimization methods such as particle swarm and cuckoo search in future research.

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