An Investigation of Pb Geochemical Behavior Respect to Those of Fe and Zn Based on k-Means Clustering Method

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Abstract

A well-known algorithm of clustering is k-means by which the data are divided into k classes based upon a distance criterion. In the present research, by using k-means method for classifying data derived from exploration boreholes in the Parkam deposit, the optimum k has been calculated and then the data have been clustered and the relative geochemical behavioral characteristics analyzed. The criterion used for determining the optimum k ranged the number of classes from k=3 to k=10 and afterwards, analyzed derived classifications in order to choose the optimum k. Results showed that clustering with k=3 in case of Pb and Zn and k=4 in case of Pb and Fe were better than other classes number in each case and according to derived classification and above cases, increase in Pb grade is followed by increase in Zn grade and also There is an increase and subsequent decrease in Fe grade. Thus, it is possible to investigate the fluctuation of elements such as Cu or Pb with other elements existing in done analysis using suggested above method that can provide a very appropriate viewpoint in front of this industry decision makers.

Keywords: k-Means, Clustering, Pb, Zn, Fe, Parkam.

1– Introduction

Considering Miduk and Parkam areas located at Kerman Copper Belt (with a length of 500 km and containing 35 porphyry systems) and the presence of copper-rich resources in the region (K.I.e.c. engineers, 2009), the necessity of determining the statistical characteristics such as mean grade value and variance and also the behavioral analysis of Cu, Mo, Pb, Zn and Fe towards one another is obvious. The geochemical data populations were resulted from exploration drilling, coring and chemical analysis in Miduk exploration area and were treated for determining initial statistical characteristics by Ghannadpour (Ghannadpour and Hezarkhani, 2012). In addition to Cu and Mo which are major ore-forming elements in porphyry systems, Pb and Zn have also been paid attention as these have significant impact on estimating the extent to which a primary geochemical halo is expanded (Gent et al., 2011). In some cases, also Pb and Zn are observed to show concentrations of ore grade (Jébrak, 2006). Hence to make a more effective estimation of geochemical halo boundaries in porphyry systems, relative behavioral characteristics of mentioned elements need to be analyzed. Thus in the present research, methods of data mining sciences were utilized for performing the analysis.

One of the most important viewpoints in data mining science concerning with analysis of large amounts of data and samples of different properties includes clustering viewpoint which is comprised of different methods and techniques as hierarchical method, k-means method, density-based methods, Kohonen’s method and many other methods that have frequently been applied in different fields of research (Devijver and Kittler, 1982;

Anderberg, 1973) by numerous researchers. Clustering assumption involves the collection M including m specimens in the form of (x_1, x_2, …, x_3), to each of which a vector in collection M is attributed and the vector represents different characteristics of the specimen (Nelson *et al.*, 2012). Assume that these specimens are to be classified into k classes or groups. For this purpose, some basic justifiability criteria must be satisfied (Jain, 2010; Pelleg and Moore, 1999). The assumptions are as follows:

$$C_i \neq \varnothing, \quad for\ i = 1,...,K \tag{1}$$

$$C_i \cap C_j = \varnothing, \quad for\ i \neq j \tag{2}$$

$$\bigcup_{i=1}^{K} C_i = M \tag{3}$$

According to the first assumption, no one of k collections must be null. The second assumption states that collections must not overlap and the third assumption states that no specimen must be out of collection.

One of the well-known and simple methods of data mining has been the k-means in which the sum of Euclidean distances of specimens to the center of associated collection must be minimized. Relative geochemical behavioral characteristics have been analyzed through different approaches (Menard, 1995; Xu *et al.*, 2012; Tarkian and Stribrny, 1999). Further in data mining literature, there are numerous studies utilizing clustering methods especially k-means for classifying the data populations associated with earth variables and often of a geochemical nature. The following can be indicated as examples: classifying land features (Yang *et al.*, 2012), classifying the effect of vegetation on water healthiness recovery in Mediterranean forests (Mora *et al.*, 2012), planning the identification of geochemical patterns in mining districts applying k-means method (Meshkani *et al.*, 2011), organic carbon prediction by intelligent systems comparing k-means and intelligent methods (Sfidari, *et al.*, 2012), and determining the gas emission effect in urban environments applying clustering analysis by k-means method (Wegner, *et al.*, 2012). Moreover, there have been researches applying k-means with advanced innovative algorithms which yielded favorable results (Krishna and Narasimha Murty, 1999; Cheung, 2003; Murthy and Chowdhury, 1996). Yaghini (Yaghini *et al.*, 2008) devised a combined clustering method (GKA) engaging both genetic and k-means algorithms. The latter method utilizes k-means Operator which is designed based upon k-means algorithm (Yaghini *et al.*, 2008).

2– K-Means Algorithm

One of the well-known viewpoints in data mining has been the k-means clustering method which starts with a certain number of collections (k) and clusters specimens into these k group so that the assumptions 4 and 5 are satisfied (Saha and Bandyopadhyay, 2012). The criterion based upon which specimens are attributed to collections is the minimum Euclidean distance between each specimen and the central point (representative point) of each group. The most important stages of k-means algorithm have been defined by Yi (Yi and Zhang, 2012) and Jain (Jain, 2010) as follows:

1. Introducing k class or group as (C_1, C_2, …, C_k) in order for clustering m specimens from the collection M.

2. Calculating the vector zj (based on equation 4) which is representative of each class Cj.

$$z_j = \frac{\sum_{x \in C_j} x}{\# C_j} \qquad for\ j = 1, 2..., K \tag{4}$$

The parameter x in equation 4 stands for the vector of a specimen which is a member of Cj and #Cj stands for the number of specimens that are members of Cj (this equation is used for calculating the class central points while solving the algorithm begins with random number of specimens (k) and attributes them to the center of each group.

3. Calculating of the objective function derived from classification (C_1, C_2, …, C_k) based on equation (5) which calculated the sum of distances between specimens and central point.

$$f(C_1, C_2, ..., C_K) = \sum_{j=1}^{K} \sum_{x \in C_j} \|x - j\|^2 \quad (5)$$

4. Minimizing objective function and determining appropriate classification for collection M with k number of classes. The operation procedure is illustrated in Figure 1.

1. ***Let $C_1, C_2, \dots, C_k$ be a set of k clusters of M.***
2. ***Let $Z_j = (\sum_{x \in c_j} x)/\#C_j$ for $j = 1, 2, \dots, k$, where x is a pattern vector in C_j and $\# C_j$ represents the number of points in C_j.***
3. ***Let $f(C_1, C_2, \dots, C_k) = \sum_{j=1}^{k} \sum_{x \in C_j} |x - z_j|^2$. we shall refer to $f(C_1, C_2, \dots, C_k)$ as the objective function of the clustering $C_1, C_2, \dots, C_k$.***
4. ***Minimize $f(C_1, C_2, \dots, C_k)$ over all $C_1, C_2, \dots, C_k$ satisfying P_1, P_2 and P_3 stated in Section 1.***

Figure 1) Performance of k-Means Algorithm (Yaghini et al., 2008).

3– Regional Geology

A dozen porphyry copper occurrences occur in the southeastern sector of the central Iranian Cenozoic magmatic arc from which the middle/late Miocene diorite-type of Parkam, Miduk and granodiorite-type of Sarcheshmeh are some well-known systems. These porphyry copper deposits are located in south southeast central Iran in the elongated NW-trending median mountain range of Kerman Province. The Parkam and Sarcheshmeh deposits are located at latitudes 30° 27' 27" and 29º 56' 55" N, and longitudes 55º 8' 8" and 55º 52' 28" E, respectively (Fig. 2). A faulted and gently folded upper Eocene-Oligocene complex of poorly bedded lavas, volcanoclastic rocks, and subordinate sedimentary deposits constitute the country rocks to the Neogene intrusions.

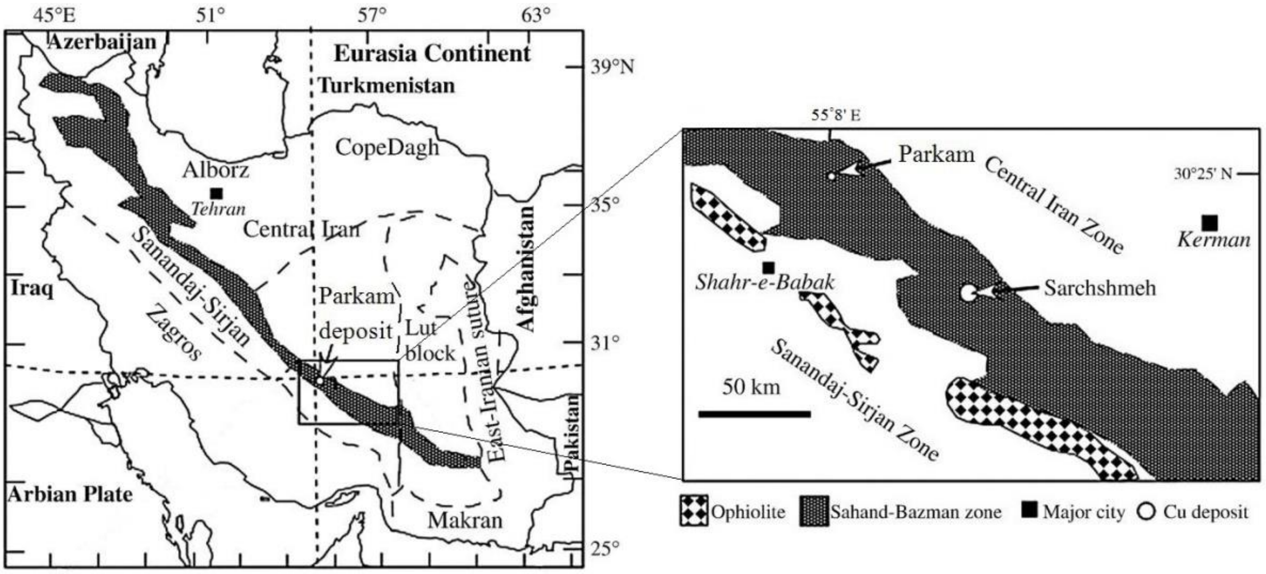

Figure 2) Map showing major litho-tectonic structural zones of Iran. Enlarged part shows location of the Parkam porphyry Cu deposit, the giant Sarcheshmeh porphyry Cu–Mo deposit and the city of Shahr-e-Babak. Stippled zone is Sahand–Bazman (modified after Berberian and King, 1981).

The small Parkam stock is a part of the Sahand-Bazman igneous and metallogenic belt (northern Iran), a deeply eroded Tertiary volcanic field, roughly 100 by 1700 km in extent (from Turkey to Baluchistan in southern Iran (Hezarkhani, 2008)), consisting mainly of rhyolite and andesite, with numerous felsic intrusions (Fig. 3). The litho-tectonic units illustrated in Figure 3 formed as a result of the opening and closing of the Paleo–Tethys and Neo–Tethys oceanic basins, due to subduction and terminal collision and transpression events. To the north, Iran collided with Turkmenistan or Turan plate (Eurasia) in the late Triassic–early Jurassic period (Berberian and King, 1981). In the south, Iran experienced subduction and collided with the Arabian plate in the Late Cretaceous (Berberian and King, 1981; Takin, 1972; Stocklin, 1974; Stocklin, 1977; Hallam, 1976; Welland and Mitchell, 1977; Adamia *et al.*, 1980). Arc magmatism continued through the Miocene and Late Neogene (Alavi, 1994; Walker and Jackson, 2002; Shahabpour, 2005) which resulted in extensive alkaline and calc-alkaline volcanic and plutonic igneous activity (Etminan, 1978; Shahabpour, 1982; Berberian, 1983; Hezarkhani, 2006a; Hezarkhani, 2006b), including the Miocene intrusion of a porphyritic calc-alkaline stock at Parkam (Shahabpour, 1982). The volcanics were laid down unconformably over folded and eroded Upper Cretaceous andesitic volcanic and sedimentary rocks (~500 m thick).

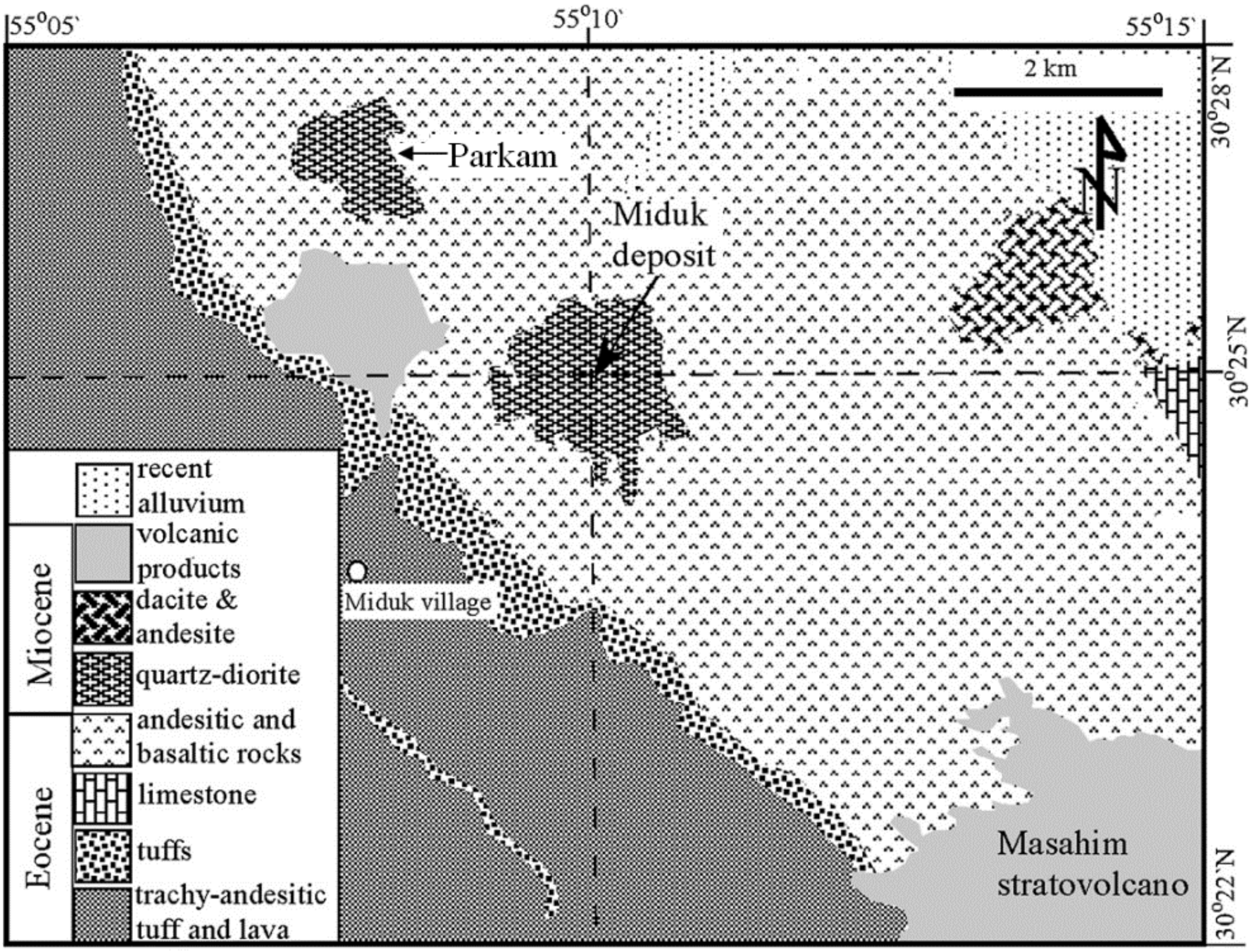

Figure 3) Regional geological map of the Parkam area, based on the geological map of Shahr-e-Babak (modified after Saric et al., 1971).

3.1- Geological Setting of Parkam Porphyry Copper System

Parkam exploration field having an area of 4 km^2 is located approximately 50 km north of Shahr-e-Babak. The area lies at 1:100000 geological map of Shahr-e-Babak and 1:250000 geological map of Anar.

Lithological units of the deposit area are predominantly Eocene volcanic rocks. Additionally, northwest and central parts of the Shahr-e-Babak region are comprised of Eocene sedimentary rocks and Neogene pyroclastic rocks. In addition, a vast area of Shahr-e-Babak region is comprised of coarse-grained alluvial sediments of Quaternary period. The geological map of the Parkam area is shown in Figures 2 and 3. Geological units in the deposit area have been described as follows:

Cretaceous: There are several outcrops of Colored Melange existing as accumulations of serpentinite to gabbroic rocks at western parts of the area. These minor outcrops are to be the oldest rocks of the area (P.O.E. Consultant, 2009).

Eocene: Early Eocene strata are Flysch, conglomerate, red sandstone, limestone and limy to marly sedimentary units chronologically. The oldest formation of Eocene, the Flysch sedimentary unit which contains outcrops of Eocene Conglomerate units and are intersected by some dykes. Moreover, there are outcrops of Eocene red Sandstone and Marl units in Eocene volcanic rocks (P.O.E. Consultant, 2009). The late Eocene is generally comprised of volcanic rocks which have been described as follows chronologically:

(1) andesitic basalts of a few hundred meters thickness; (2) red tuffs and tuff sediments of 60 meters thickness; (3) A horizon of trachyandesite and trachybasalt rocks; (4) tuff and tuff sandstone of 70 meters thickness with a 1 meter-thick bed of Lime lying beneath which is overlain by approximately 10 meters of ignimbrite itself; (5) Trachyandesite and Trachybasalts along with basaltic lavas and agglomerate; (6) Porphyritic rocks having phenocrysts of plagioclase, monoclinic pyroxene and olivine and a matrix of plagioclase, pyroxene, feldspar and microliths (K.I.e.c. engineers, 2009).

Neogene: Early Neogene strata are comprised of red layers of sandstone and andesitic agglomerate. The sandstone layers can be observed in a small part of northwest of the area and the andesitic agglomerates which are younger than Eocene volcanic have outcrops in some parts of the area as well (P.O.E. Consultant, 2009). Middle Neogene strata are comprised of volcanic rocks of Neogene. The Masahim stratovolcano which occupies a vast area of the region is predominantly comprised of Neogene volcanic rocks and some pyroclastic cones are observed in the northern parts. The Neogene volcanic sequence begins with pyroclastic materials which have been stratiform-deposited and are followed by dacite, biotite and augite-bearing hornblende dacitoid and andesite rocks. Conglomerate and volcanic sandstone units also overlie pyroclastics and spread over several large areas. There are also hornblende andesite rocks of 20 meters thickness (P.O.E. Consultant, 2009). The late Neogene rocks are comprised of altered rocks, diorites and conglomerates. A large amount of altered rocks are comprised of volcanic rocks of Masahim stratovolcano. The altered rocks contain sulfide minerals and the altered rocks of Miduk district formed with Neogene volcanic rocks. The conglomerate units of late Neogene are also observed at two small areas of the west part of Shahr-e-Babak (K.I.e.c. engineers, 2009).

Quaternary: There is a vast land of Quaternary deposits formed at northern areas of Shahr-e-Babak as well as covers of sandstone and alluvial fan (P.O.E. Consultant, 2009).

4– Case Study

The geochemical data derived from explorations in Parkam area were analyzed applying k-means clustering method. Recently, Iran's Copper National Corporation has performed drilling, coring and chemical analysis in Parkam area. The data were resulted as Zn, Pb and Mo grade values in ppm and both Fe and Cu in weight percent (Ghannadpour and Hezarkhani, 2012). Each meter of drilling in each borehole (in this analysis considered as a sample vector (x) in the drilling collection of ICNC including several tens of thousands of meters) is considered as a vector with characteristics as Zn, Pb, Mo, Fe and Cu grade values, analysis based on each of which might provide suitable perspective for decision making. For instance, some classifications beneficial for geochemical explorations could be as follows:

a) Copper variations relative to Zn.
b) Copper variations relative to Mo.
c) Molybdenum variations relative to Fe.
d) Copper variations relative to Pb.
e) Etc.

In this section, for instance, Pb grade variations relative to Zn and Fe which are from very important elements in determining extent and spread of primary geochemical halos is considered for clustering in the way of doing behavioral analysis.

In present research, the appropriate number of classes (k) was selected by ranging k from 3 to 10 and analyzing the derived classifications. For evaluating the groups resulted from different values of k, a suitability equation for examining the classifications has been applied following (Yaghini *et al.*, 2008):

$$S(i) = \frac{Min(AVEG\_BETWEEN(i,k)) - AVEG\_WITHIN(i)}{Max[AVEG\_WITHIN(i), Min(AVEG\_BETWEEN(i,k))]} \quad (6)$$

The parameter S(i) in the equation (6) represents the suitability of the ith indexed specimen in its associated class, the parameter "AVEG_WITHIN(i)" stand for the average distance between the ith specimen and the rest of specimens in a particular class and the parameter "AVEG_BETWEEN(i,k)" represents the average distance between the ith specimen and specimens present in an alternative class as k (Yaghini *et al.*, 2008).

According to equation (6), suitability can range between -1 (inappropriate classification) and +1 (appropriate classification). Also 0 implies in difference for the specimen being classified either in associated class or else.

4.1- Geochemical behavior analysis of Pb relative to Zn

Figure 4 represents the silhouette value that indicates the suitability of each specimen of Pb and Zn case testing with 3 and 4 classes (k).

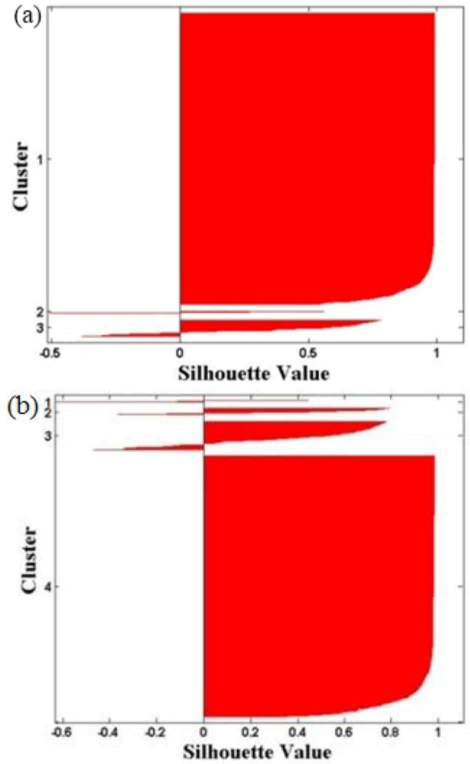

Figure 4) Classes silhouette and suitability value for classification relating to Pb and Zn. a) Classification with k=3, average value of 0.9283; b) Classification with k=4, average value of 0.8759.

As represented, the classes 1 and 2 have appropriate silhouette values for k=3 and there are nearly few negative silhouette values associated with class 2. Additionally, the average silhouette value is 0.9283. There are also negative silhouette values in k=4 testing (having an average silhouette value of 0.8218). Obviously, clustering with k=3 is preferred to k=4 (due to the greater value of average silhouette). The same is performed for k=5 to k=10 cases (Fig. 5).

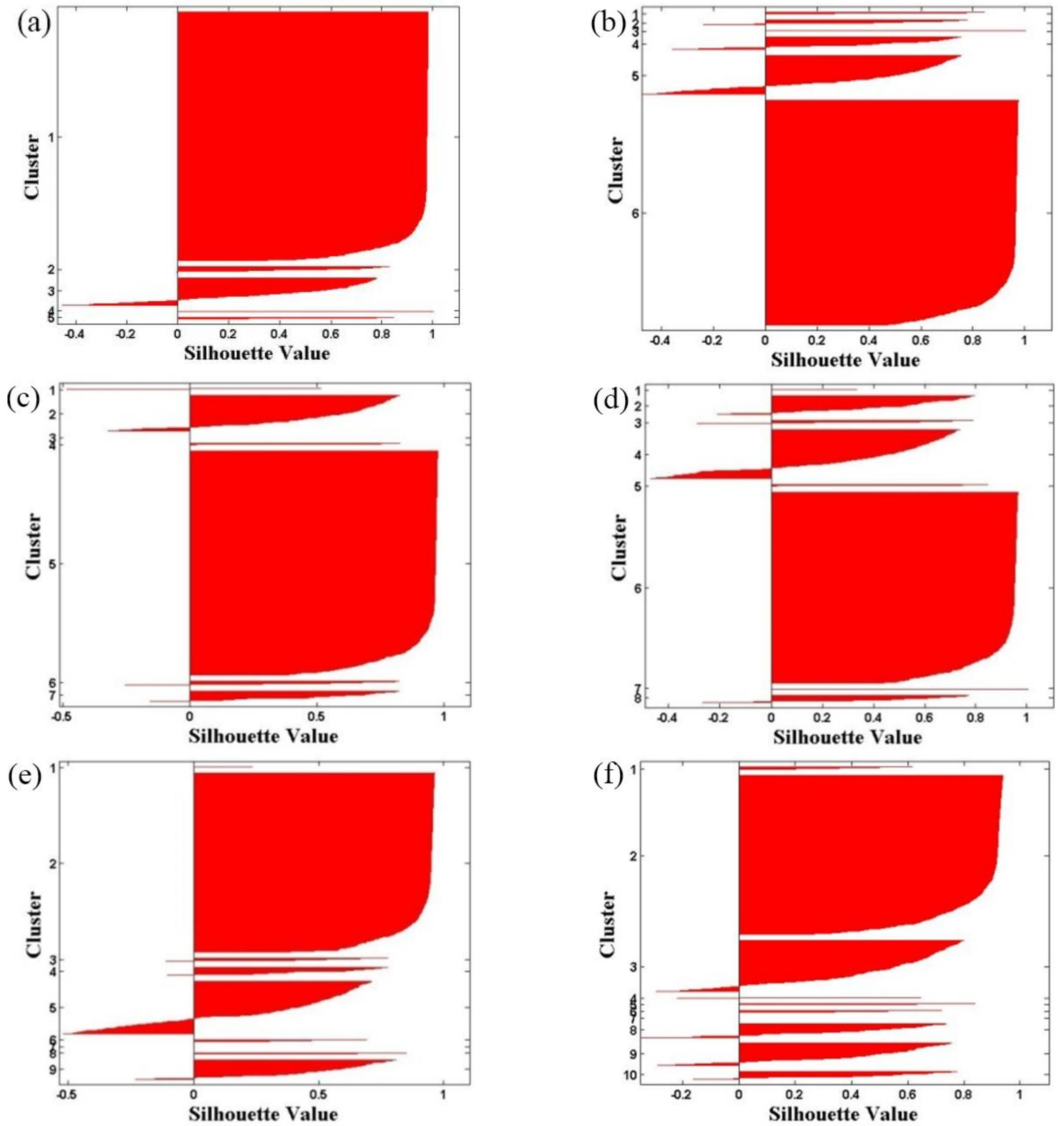

Figure 5) Classes silhouette and suitability value for classification relating to Pb and Zn. a) Classification with k=5, average value of 0.8829;(b) Classification with k=6, average value of 0.814; c) Classification with k=7, average value of 0.8373; d) Classification with k=8, average value of 0.7657; e) Classification with k=9, average value of 0.7226; f) Classification with k=10, average value of 0.7105.

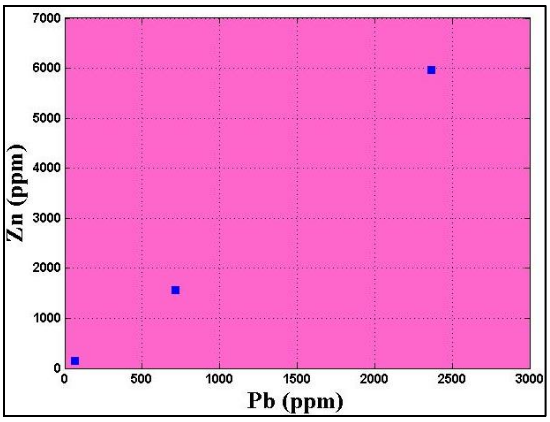

Figure 6) The central points of the k=3 classification relating to Pb and Zn.

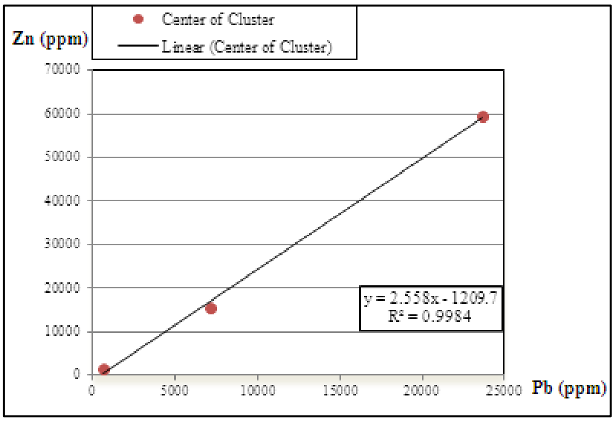

Figure 7) Regression line crossed from classes central point relating to Pb and Zn.

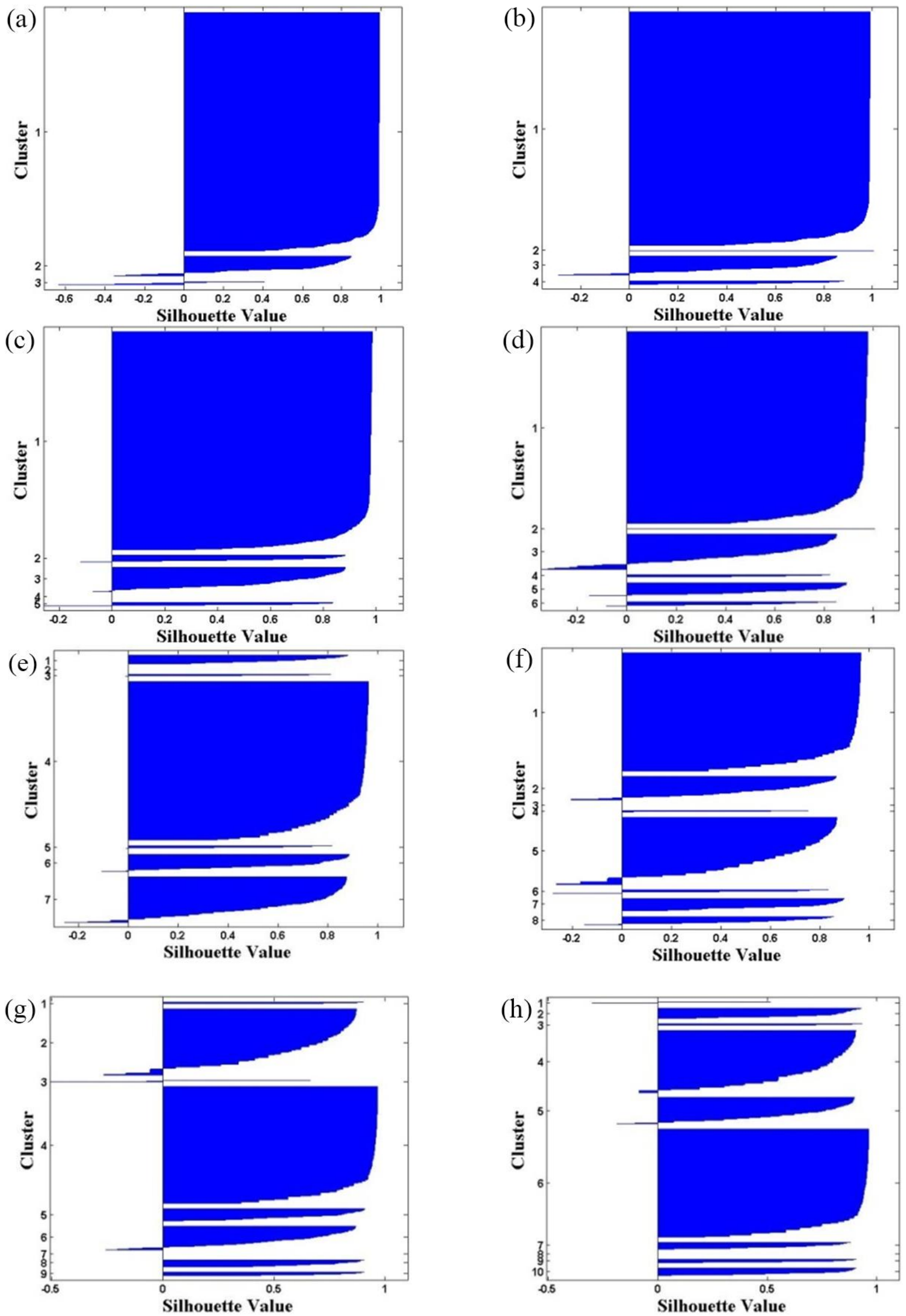

Figure 8) Classes silhouette and suitability value for classification relating to Pb and Fe. a) Classification with k=3, average value of 0.9167; b) Classification with k=4, average value of 0.9296; c) Classification with k=5, average value of 0.9042; d) Classification with k=6, average value of 0.8394; e) Classification with k=7, average value of 0.7966; f) Classification with k=8, average value of 0.7395; g) Classification with k=9, average value of 0.7491; h) Classification with k=10, average value of 0.7772.

Eventually, considering the results for k=3 to k=10, clustering with k=3 for the specimens of Pb and Zn grade attributes was selected. The central points of the k=3 classification are represented in Figure 6. As illustrated, Zn grade varies linear relative to Pb grade values. The best regression was $y = 2.558x \pm 1209.7$ and the correlation coefficient was reported $R^2 =$

0.9984 by MATLAB software. Figure 7 represents regression line fitted to class central points of Pb and Zn case.

4.2- Geochemical behavior analysis of Pb relative to Fe

Figure 8 represents the silhouette value which indicates the suitability of each specimen presented in classification with k=3 to k=10 in the case of Pb and Fe. The considering the result derived from analysis with k=3 to k=10, as illustrated, the classification with k=4 for specimens having characteristics of Pb and Fe grade values best satisfies the criteria of data mining suggested above (see equation 6). The central points of classes derived from clustering with k=4 are represented in Figure 9.

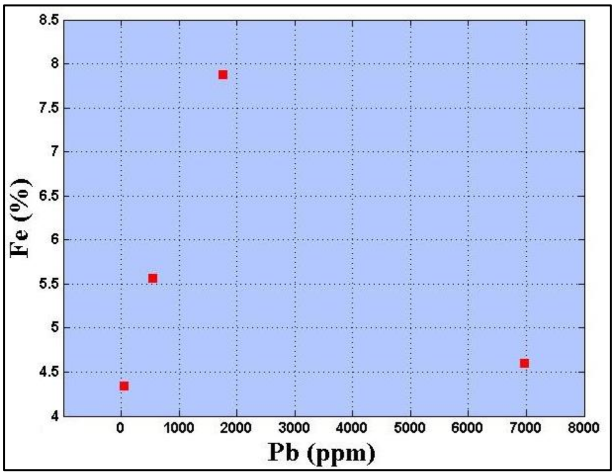

Figure 9) The central points of the k=4 classification relating to Pb and Fe.

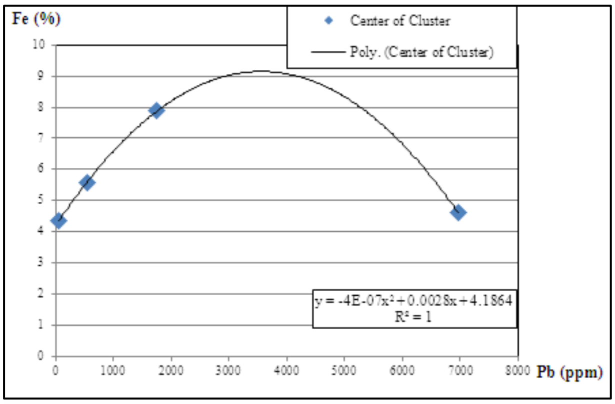

Figure 10) Regression curve fitted to classes central points relating to Pb and Fe.

Considering Figure 10, increasing Pb grade values, causes an increase and a subsequent decrease in Fe grade values. According to this fluctuation, best regression curve is in order 2 and negative concavity. Anyway, the curve fitted on central points by MATLAB software was $y = -4 \times 10^{-7}x^2 + 0.0028x + 4.1864$ and the correlation coefficient was reported as $R^2 = 1$.

5– Conclusions

Considering Miduk and Parkam area located at Kerman Copper Belt (500 km length and containing at least 35 porphyry deposits) and the plenty of copper-rich resources present there, the necessity of knowledge on the quality of behavior including relative geochemical behavior seems obvious. This information would assist in locating and magnifying the geochemical halos of porphyry systems, deciding whether an area is worth further exploration and estimating the mean grade value. Thus in present study k-means clustering method was applied for classifying the geochemical dataset derived from exploration drillings over Parkam area. One of the problems commonly encountered in cases that a huge amount of data involving large number of classes is clustered using k-means algorithm is Local Optimized Spot which has not been troubling here due to the slim amount of data being clustered in this study. The k-means method includes the k parameter which is the number of classes and must be selected optimally. Thus in this study, there has been an appropriate criterion defined for determining optimal k. The final results are as follows:

a) In Pb and Zn case, for k values ranging from 3 to 10, clustering with k=3 was relatively more suitable and the best silhouette value in this case was 0.9296.
b) There are increasing Zn grade values growing with increasing Pb grade values in the area. The equation of fitted curve is $y = 2.558 \pm 1209.7$. The correlation coefficient of equation fitted to the class central points is $R^2 = 0.9984$.

c) In Pb and Fe case, for k values ranging from 3 to 10, clustering with k=4 was relatively more suitable and the best silhouette value in this case was 0.9283.

There is an increase and subsequent decrease in Fe grade values with growing grade values of Pb. According to this fluctuation, best regression curve is in order 2 and with negative concavity. Anyway, the curve fitted on central points by MATLAB software was $y = -4 \times 10^{-7}x^2 - 0.0028x + 4.1864$ and the correlation coefficient was reported as $R^2 = 1$.

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