

Fuzzy Hierarchical Cross-Classification of Greek Muds

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In this paper we analyze the set of Greek muds from eight different locations given in ref 16 using a divisive fuzzy hierarchical cross-classification algorithm. We consider the fuzzy clustering algorithms are capable to eliminate the disfunctionalities of the hard clustering algorithms as well as to provide information obtained from a metrical analysis of the data. The fuzzy hierarchical cross-classification algorithm presented here produces not only a fuzzy partition of the muds in discussion but also a fuzzy partition of the 23 chemical and mineralogical characteristics, so that to each class of muds we may associate the class of characteristics that contributed to the separation of the class of muds.

1. INTRODUCTION

Muds have been used empirically, nonetheless effectively, since the antiquity. However, it was not until 1931 that the International Society of Medical Hydrology established certain criteria for muds' classification and their corresponding therapeutic practices.

Forty mud and pelloid samples were collected from eight different locations during summer 1990. The data presented in Table 1 represent the analysis of one sample considered to be the most representative (see ref 16) for each location.

There are two opposite approaches to hierarchical clustering, namely *agglomerative* and *divisive* procedures. An agglomerative hierarchical classification places each object in its own cluster and gradually merges the clusters into larger and larger clusters until all objects are in a single cluster. The divisive hierarchical clustering reverses the process by starting with all the objects in a single cluster and subdividing it into smaller ones until, finally, each object is in a cluster of its own. The number of clusters to be generated may be either specified in advance or optimized by the algorithm itself according to certain criteria.

The fuzzy sets theory, developed by Zadeh,²³ allows an object to belong to many clusters with different membership degrees. The membership degree of an object to a certain class is supposed to be gradual rather than abrupt (either 0 or 1), revealing a basis for considering uncertainty and imprecision.

Blaffert² and Otto and Bandemer^{1,17,18,19} have considered fuzzy sets theory in analytical chemistry. The applications have been focused on solving pattern recognition problems,^{2,17} multicriteria optimization, calibration of analytical methods,^{17,19} and on the design of fuzzy expert systems for selection of analytical procedures.¹ The fuzzy divisive hierarchical clustering method proposed in ref 3 has been used for acrylonitrile selectivity,^{10,14,15} for mineral waters classifications,⁷⁻⁹ for the selection and the optimal combination of solvents,^{22,12} and for the classification of Roman pottery.²¹

In the present paper the fuzzy hierarchical cross-classification algorithm (see also ref 5) is used for the nonsupervised classification of the eight muds.

2. HIERARCHICAL CROSS-CLASSIFICATION

In certain situations the number of characteristics is very big. The design of a hierarchical classifier may be simplified if at every node is used only a small subset of the characteristics, enough for the classification decision at that node. So, at every step of the hierarchical classification process we determine a fuzzy partition of a certain class and the relevant characteristics for each of the subclasses obtained. Thus, it appears the necessity of classifying both the objects and the characteristics. This classification process will be called cross-classification (or simultaneous classification).

In what follows we will present a method which allows us to obtain an objects hierarchy and a characteristics hierarchy, so that the two hierarchical classifications should correspond to each other. The method we have in mind is iterative, and the classification is done alternatively on the data set and on the characteristics set, until we will obtain two "compatible" classifications.

Fuzzy Set and Fuzzy Partition. Let us consider a set of objects $X = \{x^1, \dots, x^p\}$, these objects being characterized so that it is possible to define a measure of their (di)similarity. We need to find the partition $\{A_1, \dots, A_n\}$ of X , with $1 \leq n < p$ so that the objects members of the same class should be as similar as possible, and the objects members of different classes should be as different as possible.

One of the main difficulties of finding some classification theories is that the most classes of real objects do not have sharp boundaries. These classes may partially overlap. A certain object may have hybrid characteristics, that should put it in many classes simultaneously. This difficulty is solved if we allow for each point to be a member of each class with a certain subunitary membership. In this situation a class of objects may be described as a fuzzy set. The theory of fuzzy sets was introduced in 1965 by Lotfy A. Zadeh²³ as a natural generalization of the classical set concept. The classification structure of a set X of objects may thus be represented by a fuzzy partition of X .

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Let x^j be a certain point of the given set X . We suppose that x^j is characterized by the values of s characteristics, x_k^j , with $1 \leq k \leq s$, where x_k^j is the value of the k th characteristic of the j th point.

A fuzzy set on X is a mapping $A: X \rightarrow [0, 1]$. The value $A(x)$ represents the *membership degree* of the point $x \in X$ to the class A .

As usually, we denote the empty fuzzy set by ϕ , that is $\phi(x) = 0$ for any x in X .

The fuzzy set having the membership degree equal to 1 is also denoted by X , that is $X(x) = 1$, for any x in X .

The equality of the fuzzy sets A and B is determined by the equality condition for functions:

$$A = B \Leftrightarrow A(x) = B(x), \forall x \in X$$

The union and the intersection of the fuzzy sets may be defined in many ways. In this paper we consider the following definitions:

$$(A \cup B)(x) = \min(1, A(x) + B(x)), \forall x \in X$$

and

$$(A \cap B)(x) = \max(0, A(x) + B(x) - 1), \forall x \in X$$

It may be proved (see ref 6) that the considered definitions of \cup and \cap are the unique ones for which the following equivalence holds:

$$\left. \begin{array}{l} A \cup B = X \\ A \cap B = \phi \end{array} \right\} \Leftrightarrow A(x) + B(x) = 1, \forall x \in X$$

This means that these definitions lead to a natural definition of a fuzzy partition.

Let A , B , and C be fuzzy sets on X . $P = \{A, B\}$ is a fuzzy partition of C if the following conditions are fulfilled:

1. $A \cup B = C$
2. $A \cap B = \phi$

It is easy to note that this definition is equivalent with

$$A(x) + B(x) = C(x), \forall x \in X$$

Fuzzy Substructure of a Fuzzy Set. If the data set X is composed of two classes, then the cluster structure of the set X is described by two disjoint fuzzy sets having the union equal to X . Each fuzzy set corresponds to a class (or cluster) of points in X . The disjointness condition is a minimal separation condition of the respective classes.

We will consider a hierarchical classification scheme where the cluster structure of the data set X is given by a binary fuzzy partition. Let $\{A_1, A_2\}$ represent such a fuzzy partition. It is possible for the class A_i , $i = 1, 2$, to have a cluster substructure. We may imagine this substructure as a fuzzy partition $\{A_{i,1}, A_{i,2}\}$ of A_i . In this case, $A_{i,1}$ and $A_{i,2}$ represent subclusters of A_i .

So, we are entitled to search for the cluster substructure of a certain fuzzy set, and let us denote it by C . Let us suppose that the binary fuzzy partition corresponding to this substructure is $\{A_1, A_2\}$. We admit that each class A_i may be represented by a prototype L^i from the representation space, R^s . If L^i is from X we may suppose that L^i has the greatest membership degree to A_i , that is

$$A_i(L^i) = \max_{x \in X} A_i(x) \quad (1)$$

Let us denote by d a distance in the space R^s . For example, we may consider the distance induced by the norm of the space.

The dissimilarity $D_i(x^j, L^i)$ between a point x^j and the prototype L^i is defined as the square distance to the class A_i and is interpreted as a measure of the inadequacy of the representation of the point x^j by the prototype L^i .

If L^i is not a point from the data set X , then we have from refs 5 and 3 that

$$D_i(x^j, L^i) = (A_i(x^j))^2 d^2(x^j, L^i) \quad (2)$$

The inadequacy between the fuzzy partition P and its representation, $L = \{L^1, L^2\}$ is given by the following function

$$J(P, L) = \sum_{i=1}^2 \sum_{j=1}^p (A_i(x^j))^2 d^2(x^j, L^i) \quad (3)$$

$J(P, L)$ may also be interpreted as the representation error of P by L .

Let us observe that J is a criteria function of the type of square errors sum. The classification problem becomes the determination of the fuzzy partition P and its representation L for which the inadequacy $J(P, L)$ is minimal. Let us note that, intuitively, to minimize J means to give small membership degrees to A_i for those points in X for which the dissimilarity to the prototype L^i is large, and vice versa.

Now let us generalize the problem by considering that the fuzzy substructure of the fuzzy set C is given by a fuzzy n -partition, and let us suppose that $P = \{A_1, \dots, A_n\}$ is this partition. If we admit that d is a distance induced by the norm, we may write

$$J(P, L) = \sum_{i=1}^n \sum_{j=1}^p (A_i(x^j))^2 \|x^j - L^i\|^2 \quad (4)$$

If the norm is induced by the inner product, we have

$$\|x^j - L^i\|^2 = (x^j - L^i)^T M (x^j - L^i)$$

where M is a symmetrical and positively defined matrix. The transposing operation was denoted by T .

The criteria function becomes

$$J(P, L) = \sum_{i=1}^n \sum_{j=1}^p (A_i(x^j))^2 (x^j - L^i)^T M (x^j - L^i) \quad (5)$$

Because an algorithm to obtain an exact solution of the problem (5) is not known, we will use an approximative method in order to determine a local solution. The minimum problem will be solved using an iterative (relaxation) method, where J is successively minimized with respect to P and L .

Supposing that L is given, the minimum of the function $J(\cdot, L)$ is obtained^{5,3} for

$$A_i(x^j) = \frac{C(x^j)}{\sum_{k=1}^n d^2(x^j, L^k)}, i = 1, 2, \dots, n; j = 1, 2, \dots, p \quad (6)$$

For a given P , the minimum of the function $J(P, \cdot)$ is obtained for

$$L^i = \frac{\sum_{j=1}^p (A_i(x^j))^2 x^j}{\sum_{j=1}^p (A_i(x^j))^2}, i = 1, 2, \dots, n \quad (7)$$

We observe^{5,3} that L^i is the weighting center of the class A_i .

The iterative procedure for obtaining the cluster substructure of the fuzzy class C is called generalized fuzzy n-means (GFNM).³ Essentially, the GFNM algorithm works with Picard iterations using the relations (6) and (7). The iterative process begins with an arbitrary initialization of the partition P . The process ends when two successive partitions are close enough. To measure the distance between two partitions, we will associate to each partition P a matrix Q with the dimensions $n \times p$. Q is named the representation matrix of the fuzzy partition P and is defined as

$$Q_{ij} = A_i(x^j), i = 1, 2, \dots, n; j = 1, 2, \dots, p \quad (8)$$

Considering that Q_1 and Q_2 are the representation matrices of the partitions P_1 and P_2 , we may define

$$d(P_1, P_2) = \|Q_1 - Q_2\| \quad (9)$$

where $\|Q\| = \max_{i,j} |A_i(x^j)|$.

The process ends at the r th iteration if

$$d(P_r, P_{r+1}) < \epsilon \quad (10)$$

where ϵ is an admissible error (usually, 10^{-5}).

For $C = X$ this procedure is the well-known algorithm fuzzy n-means (FNM).³

The Problem of Inequal Size Clusters. There is one more problem. Generally, the classes have different dimensions. If we consider a small class situated near a larger one, some points from the larger class will be captured by its small neighbor. This situation may be eliminated if we use an adaptive distance (see ref 3). This distance, being influenced by the dimension of classes, will annihilate the effect of migration of peripheral points. We define the radius r_i of the fuzzy class A_i as

$$r_i = \max_{x \in X} d_i(x, L^i) = \max_{x \in X} A_i(x) d(x, L^i) \quad (11)$$

We will define the local adaptive distance, d_{ia} , as

$$d_{ia}(x, L^i) = \frac{d_i(x, L^i)}{r_i} \quad (12)$$

and the new dissimilarity as

$$D_i(x^j, L^i) = d_{ia}^2(x^j, L^i) \quad (13)$$

The criteria function becomes

$$J(P, L) = \sum_{i=1}^2 \sum_{j=1}^p (A_i(x^j))^2 \frac{d^2(x^j, L^i)}{r_i^2} \quad (14)$$

By using the adaptive distance, the problem of unequal clusters will not appear, because the radii of the two clusters are equal.

POLARIZATION AND FUZZINESS

Because the optimal number of classes generally is not known, we will use a divisive hierarchical clustering procedure. The problem that appears now is to decide whether a class may be divided or not.

Let us suppose that the fuzzy class C was divided in the two fuzzy classes C_1 and C_2 . If C describes an homogenous cluster, the membership degrees of trend to be uniform (the majority of points will have the membership degrees of about $C(x)/2$). On the contrary, if C contains two classes relatively well separated, this will induce a trend of polarization of the membership degrees (the majority of points will have the membership degrees polarized near the extreme values, 0 and $C(x)$).

So, the polarization of the membership degrees may be associated with the presence of a certain structure in the data set. The polarization degree of a binary fuzzy partition may be considered as measuring the partition quality. The polarization degree of P may be defined^{3,5} as

$$R(P) = \frac{\sum_{x \in X} \max(C_1(x), C_2(x))}{\sum_{x \in X} C(x)} \quad (15)$$

For example, let us consider $X = \{x^1, x^2, x^3, x^4\}$ and the fuzzy partition $P = \{A_1, A_2\}$ of X given by

| | x^1 | x^2 | x^3 | x^4 |
|------------|-------|-------|-------|-------|
| $A_1(x^j)$ | 0.9 | 0.2 | 0.7 | 0.6 |
| $A_2(x^j)$ | 0.1 | 0.8 | 0.3 | 0.4 |

In this case we have $R(P) = (0.9 + 0.8 + 0.7 + 0.6)/4 = 3/4 = 0.75$.

Let us consider now the fuzzy partition $Q = \{A_{11}, A_{12}\}$ of A_1 given by

| | x^1 | x^2 | x^3 | x^4 |
|---------------|-------|-------|-------|-------|
| $A_{11}(x^j)$ | 0.2 | 0.1 | 0.6 | 0.4 |
| $A_{12}(x^j)$ | 0.7 | 0.1 | 0.1 | 0.2 |

We have $R(P) = (0.7 + 0.1 + 0.6 + 0.4)/(0.9 + 0.2 + 0.7 + 0.6) = 1.8/2.4 = 0.75$.

If $R(P)$ is large enough ($R(P) \geq t$, where t is an appropriate threshold) we will say that the fuzzy partition P describes real clusters.

Fuzzy Divisive Hierarchical Clustering. Using the FNM algorithm we may determine a binary fuzzy partition $\{A_1, A_2\}$ of the data set X . If the partition does not describe real clusters (that is, the polarization degree, $R(P)$ is small), the data set X does not have a substructure. If this partition describes real clusters, we denote $P^1 = \{A_1, A_2\}$. Using the GFNM algorithm for two subclasses ($n = 2$) we may determine a binary fuzzy partition for each A_i of P^1 . If this partition of A_i describes real clusters, these clusters will be attached to a new fuzzy partition, P^2 . Otherwise, A_i will remain undivided. The class A_i will be marked and will be allocated to the partition P^2 .

The unmarked class members of P^2 will follow the same procedure. The divisive procedure will stop when all the classes of the current partition P^l are marked, that is there are no more real clusters.

The fuzzy hierarchy obtained is richer in information (see ref 11) than a hierarchy based on classical sets, but sometimes is useful to have a classical partition also. For a complete discussion on the problem of passing from fuzzy partitions to classical partitions, see [11]. We will only show the method used here for obtaining a classical partition.

INTERPRETATION OF THE FINAL FUZZY PARTITION

Defuzzification of the final fuzzy partition will be obtained using the maximum membership rule or a hierarchical assignment rule. This latter rule means that the classical sets corresponding to the fuzzy classes will be built simultaneously with the respective fuzzy classes, based on the following:

1. initially, $\forall x \in X, x \in \tilde{X}$
2. when we build the fuzzy partition $\{C_1, C_2\}$ of the fuzzy set C , we will say that

$$x \in \tilde{C}_1 \Leftrightarrow x \in \tilde{C} \text{ and } C_1(x) \geq C_2(x)$$

and

$$x \in \tilde{C}_2 \Leftrightarrow x \in \tilde{C} \text{ and } C_1(x) < C_2(x)$$

Remark. It is obvious that $\{\tilde{C}_1, \tilde{C}_2\}$ is a hard partition of the classical set \tilde{C} .

Finally, when obtaining the fuzzy hierarchy of the set X , we will also obtain the so-called classical hierarchy associated to the respective fuzzy hierarchy.

To conclude, the fuzzy divisive hierarchical clustering (FDHC) procedure may be used to determine the optimal cluster substructure of the data set. This method is specially useful when the number of classes is unknown.

SIMULTANEOUS FUZZY N -MEANS ALGORITHM

Let $X = \{x^1, \dots, x^p\} \subset \mathbb{R}^d$ be the set of objects to be classified. A characteristic may be specified by its values corresponded to the p objects. So, we may say that $Y = \{y^1, \dots, y^d\} \subset \mathbb{R}^d$ is the set of characteristics. y_j^k is the value of the characteristic k with respect to the object j , so we may write $y_j^k = x_j^k$.

Let P be a fuzzy partition of the fuzzy set C of objects and Q be a fuzzy partition of the fuzzy set D of characteristics. The problem of the cross-classification (or simultaneous classification) is to determine the pair (P, Q) which optimizes a certain criterion function. By starting with an initial partition P^0 of C and an initial partition Q^0 of D , we will obtain a new partition P^1 . The pair (P^1, Q^0) allows us to determine a new partition Q^1 of the characteristics. The algorithm consists in producing a sequence (P^k, Q^k) of pairs of partitions, starting from the initial pair (P^0, Q^0) , in the following steps

- (i) $(P^k, Q^k) \rightarrow (P^{k+1}, Q^k)$
- (ii) $(P^{k+1}, Q^k) \rightarrow (P^{k+1}, Q^{k+1})$

The rationale of the hierarchical cross-classification method⁵ essentially supposes the splitting the sets X and Y in two

subclasses. The obtained classes are alternatively divided in two subclasses, and so on. The two hierarchies may be represented by the same tree, having in each node a pair (C, D) , where C is a fuzzy set of objects and D is a fuzzy set of characteristics.

As a first step we propose ourselves to simultaneously determine the fuzzy partitions (as a particular case, the binary fuzzy partitions) of the classes C and D , so that the two partitions should be highly correlated.

With the generalized fuzzy n -means algorithm, we will determine a fuzzy partition $P = \{A_1, \dots, A_n\}$ of the class C , using the original characteristics.

In order to classify the characteristics, we will compute their values for the classes $A_i, i = 1, \dots, n$. The value \bar{y}_i^k of the characteristic k with respect to the class A_i is defined as

$$\bar{y}_i^k = \sum_{j=1}^p A_i(x^j) x_j^k, i = 1, \dots, n; k = 1, \dots, d \quad (16)$$

Thus, from the original d p -dimensional characteristics we computed d new n -dimensional characteristics which are conditioned by the classes $A_i, i = 1, \dots, n$. We may admit that these new characteristics do not describe objects, but they characterize the classes A_i .

Let us consider now the set $\bar{Y} = \{\bar{y}^1, \dots, \bar{y}^d\}$ of the modified characteristics. We define the fuzzy set \bar{D} on \bar{Y} , given by

$$\bar{D}(\bar{y}^k) = D(y^k), k = 1, \dots, d$$

The way the set \bar{Y} has been obtained lets us conclude that if we will obtain an optimal partition of the fuzzy set D , this partition will be highly correlated to the optimal partition of the class C .

With the generalized fuzzy n -means algorithm we will determine a fuzzy partition $Q = \{B_1, \dots, B_n\}$ of the class D , by using the characteristics given by the relation (16).

We may now characterize the objects in X with respect to the classes of proprieties $B_i, i = 1, \dots, n$. The value \bar{x}_i^j of the object k with respect to the class B_i is defined as

$$\bar{x}_i^j = \sum_{k=1}^d B_i(\bar{y}^k) x_j^k, i = 1, \dots, n; j = 1, \dots, p \quad (17)$$

Thus, from the original p d -dimensional objects we have computed p new n -dimensional objects, which correspond to the classes of characteristics $B_i, i = 1, \dots, n$.

Let us now consider the set $\bar{X} = \{\bar{x}^1, \dots, \bar{x}^p\}$ of the modified objects. We define the fuzzy set \bar{C} on \bar{X} , given by

$$\bar{C}(\bar{x}^j) = C(x^j), j = 1, \dots, p$$

With the generalized fuzzy n -means algorithm we will determine a fuzzy partition $P' = \{A'_1, \dots, A'_n\}$ of the class C , by using the objects given by the relation (17). The process continues until two successive partitions of objects (or of characteristics) are close enough to each other. Thus, we have obtained the **simultaneous fuzzy n -means algorithm** (see ref 5).

S1. Set $l = 0$. With the generalized fuzzy n -means algorithm we determine a fuzzy n -partition $P^{(l)}$ of the class C by using the initial objects.

Table 1. Composition of the Original set of Eight Muds (the Muds Are Presented Vertically)^a

| sample | Krinides | Pikrolimni | Lisbori | Thermi | Kyllini | Black mud | Boario | Argilla Solare |
|---|----------|------------|---------|--------|---------|-----------|--------|----------------|
| Na ⁺ | 0.105 | 6.780 | 0.262 | 0.398 | 0.083 | 3.410 | 0.210 | 0.197 |
| K ⁺ | 0.024 | 0.040 | 0.072 | 0.028 | 0.016 | 0.250 | 0.152 | 0.020 |
| Ca ²⁺ | 0.021 | 0.010 | 0.234 | 0.041 | 0.085 | 0.760 | 0.060 | 0.000 |
| Mg ²⁺ | 0.006 | 0.010 | 0.035 | 0.006 | 0.013 | 0.080 | 0.011 | 0.004 |
| Cl ⁻ | 0.180 | 6.360 | 0.270 | 0.690 | 0.095 | 5.040 | 0.295 | 0.006 |
| HCO ₃ ⁻ | 0.038 | 1.020 | 0.025 | 0.022 | 0.219 | 1.950 | 0.052 | 0.135 |
| SO ₄ ²⁻ | 0.048 | 3.250 | 0.960 | 0.055 | 0.140 | 0.710 | 0.328 | 0.130 |
| NO ₃ ⁻ | 0.000 | 0.140 | 0.002 | 0.000 | 0.009 | 0.110 | 0.032 | 0.030 |
| CO ₃ ²⁻ | 0.000 | 0.910 | 0.000 | 0.000 | 0.000 | 0.270 | 0.000 | 0.114 |
| CaCO ₃ | 3.100 | 9.200 | 4.700 | 26.100 | 17.100 | 51.400 | 10.300 | 1.100 |
| MgCO ₃ | 0.400 | 3.500 | 0.700 | 0.700 | 1.000 | 5.400 | 1.100 | 0.500 |
| Fe ₂ O ₃ | 0.700 | 1.800 | 1.600 | 0.300 | 0.600 | 0.500 | 1.500 | 0.900 |
| organic | 6.500 | 2.500 | 1.800 | 0.500 | 5.500 | 1.600 | 1.800 | 0.900 |
| Ash | 85.900 | 87.100 | 90.500 | 82.200 | 83.800 | 72.100 | 88.200 | 89.800 |
| pH | 7.800 | 9.800 | 7.700 | 8.400 | 7.800 | 8.500 | 7.500 | 10.200 |
| CEC | 15.000 | 8.000 | 26.000 | 19.000 | 4.000 | 2.000 | 10.000 | 18.000 |
| Na ₂ O | 0.900 | 2.200 | 2.300 | 1.000 | 1.200 | 0.900 | 0.500 | 1.400 |
| K ₂ O | 2.800 | 2.500 | 3.000 | 1.400 | 1.100 | 0.900 | 1.600 | 3.200 |
| CaO | 0.300 | 0.300 | 1.300 | 0.600 | 1.100 | 1.600 | 1.100 | 0.200 |
| MgO | 0.800 | 1.600 | 1.300 | 0.800 | 0.800 | 0.400 | 1.600 | 4.200 |
| Al ₂ O ₃ | 14.800 | 16.300 | 16.000 | 11.100 | 7.800 | 5.300 | 16.600 | 16.900 |
| Fe ₂ O ₃ ^a | 2.700 | 4.400 | 4.100 | 4.100 | 1.800 | 2.000 | 5.200 | 6.500 |
| SiO ₂ | 60.300 | 35.600 | 56.100 | 46.700 | 58.600 | 17.100 | 52.800 | 54.500 |

^a Denotes the chemical analysis of the aluminosilicates residue.

S2. With the generalized fuzzy n -means algorithm we determine a fuzzy n -partition $Q^{(l)}$ of the class D by using the characteristics defined in (16).

S3. With the generalized fuzzy n -means algorithm we determine a fuzzy n -partition $P^{(l+1)}$ of the class C by using the characteristics defined in (17).

S4. If the partitions $P^{(l)}$ and $P^{(l+1)}$ are close enough, that is if

$$\|P^{(l+1)} - P^{(l)}\| < \epsilon$$

where ϵ is a preset value, then **Stop**, else set $l = l + 1$ and go to **S2**.

Let us denote the final partitions obtained above by $P = \{A_1, \dots, A_n\}$ and $Q = \{B_1, \dots, B_n\}$. If we will try to build the fuzzy partitions corresponding to the fuzzy sets A_i and B_i , $i = 1, \dots, n$, with the help of this algorithm, when computing for the first time the fuzzy partition of objects, instead the original objects we may use the objects defined in the relation (17) and determined before the end of the algorithm that produced the fuzzy partitions P and Q .

Now we will present the procedure of hierarchical class-classification. For this we will show the way of building the classification binary tree.

The nodes of the tree are labeled with a pair (C, D) , where C is a fuzzy set from a fuzzy partition of objects and D is a fuzzy set from a fuzzy partition of characteristics. The root node corresponds to the pair (X, Y) . In the first step the two subnodes (A_1, B_1) and respectively (A_2, B_2) will be computed by using the simultaneous fuzzy n -means algorithm. Of course, these two nodes will be effectively built only if the fuzzy partitions $\{A_1, A_2\}$ and $\{B_1, B_2\}$ describe real clusters.

For each of the terminal nodes of the tree we try to determine partitions having the form $\{A_1, A_2\}$ and $\{B_1, B_2\}$, by using the simultaneous fuzzy n -means algorithm, modified as we have mentioned before. In this way the binary classification tree is extended with two new nodes, (A_1, B_1) and (A_2, B_2) . The processes continues until for any terminal node we are not able to determine a structure of real clusters,

either for the set of objects or for the set of characteristics. The final fuzzy partitions will contain the fuzzy sets corresponding to the terminal nodes of the binary classification tree.

3. CLASSIFICATION RESULTS AND DISCUSSIONS

To illustrate the power of the present fuzzy cross-classification algorithm we refer to the data discussed by Mitrakas and Sikalidis,¹⁶ concerning the results of chemical and mineralogical analysis of Greek spring mineral muds and pelloids. The physico-chemical characteristics were determined in order to evaluate their use for therapeutic applications. The samples were selected so that they should represent deposits that either are currently used or may be used for these purposes.

Considering the results presented in Table 1, they concluded the following. Pikrolimni and Thermi samples had a pH of 9.8 and 8.4, respectively, which suggest their potential as beautifying muds. The high montmorillonite content of Lisbori and Thermi samples is also indicative for their effective application. Kyllini samples exhibited poor mud characteristics due to their low content of clay minerals and high content of silica. If Krinides deposits are to be commercially exploited, they should be beneficiated with the intent to increase their clay mineral content. Much more, samples of various well-known beautifying muds, such as "Black mud" from the Dead Sea, Israel and "Argilla Solare" from Italy as well as a maturated mud from "Boario Terme" of Italy, were also examined for comparative purposes. Their composition substantiates the fact that the desirable mud characteristics are a high amount of clay minerals, a high pH, and low amount of free silica, feldspar, and carbonates.

By applying our fuzzy cross-classification technique to the same data (8 samples \times 23 characteristics) we have obtained the results presented in the Tables 2–5. Figure 1 shows the final classification hierarchy. Tables 2 and 3 show the memberships of the samples to the final fuzzy samples partition and the memberships of the characteristics to the

Table 2. The Muds Memberships to the Final Fuzzy Muds Partition

| class | Krinides | Pikrolimni | Lisbori | Thermi | Lyllini | Black mud | Boario | Argilla Solare |
|------------|----------|------------|---------|---------|---------|-----------|---------|----------------|
| A_{111} | 0.77478 | 0.14327 | 0.13830 | 0.10597 | 0.14347 | 0.00049 | 0.20968 | 0.14460 |
| A_{1121} | 0.01401 | 0.06378 | 0.69865 | 0.05704 | 0.03344 | 0.00023 | 0.04783 | 0.00260 |
| A_{1122} | 0.02064 | 0.08708 | 0.00152 | 0.04968 | 0.04027 | 0.00024 | 0.08739 | 0.75363 |
| A_{121} | 0.05148 | 0.50674 | 0.05447 | 0.26476 | 0.05628 | 0.00086 | 0.19325 | 0.03386 |
| A_{122} | 0.11280 | 0.04198 | 0.06641 | 0.34474 | 0.63832 | 0.00071 | 0.45165 | 0.03812 |
| A_2 | 0.02628 | 0.15715 | 0.04066 | 0.17781 | 0.08821 | 0.99747 | 0.01020 | 0.02720 |

Table 3. The Characteristics Memberships to the Final Fuzzy Characteristics Partition

| class | Na ⁺ | K ⁺ | Ca ²⁺ | Mg ²⁺ | Cl ⁻ | HCO ₃ ⁻ | SO ₄ ²⁻ | NO ₃ ⁻ |
|------------|-----------------|----------------|------------------|------------------|-----------------|-------------------------------|-------------------------------|------------------------------|
| B_{111} | 0.010 19 | 0.022 61 | 0.020 29 | 0.025 40 | 0.007 82 | 0.014 70 | 0.001 87 | 0.024 62 |
| B_{1121} | 0.853 22 | 0.005 07 | 0.010 88 | 0.010 45 | 0.787 71 | 0.007 48 | 0.827 12 | 0.008 53 |
| B_{1122} | 0.134 87 | 0.963 39 | 0.960 12 | 0.954 67 | 0.202 62 | 0.970 83 | 0.168 38 | 0.957 60 |
| B_{121} | 0.000 28 | 0.002 28 | 0.002 22 | 0.002 44 | 0.000 32 | 0.001 71 | 0.000 44 | 0.002 37 |
| B_{122} | 0.000 65 | 0.004 79 | 0.004 66 | 0.005 11 | 0.000 74 | 0.003 65 | 0.000 98 | 0.004 98 |
| B_2 | 0.000 79 | 0.001 87 | 0.001 83 | 0.001 92 | 0.000 80 | 0.001 62 | 0.001 21 | 0.001 90 |

| class | CO ₃ ²⁻ | CaCO ₃ | MgCO ₃ | Fe ₂ O ₃ | organic | ash | pH | CEC |
|------------|-------------------------------|-------------------|-------------------|--------------------------------|----------|----------|----------|----------|
| B_{111} | 0.018 14 | 0.179 06 | 0.027 82 | 0.089 77 | 0.771 70 | 0.007 63 | 0.149 72 | 0.029 23 |
| B_{1121} | 0.003 68 | 0.033 85 | 0.947 34 | 0.846 46 | 0.159 93 | 0.003 63 | 0.038 51 | 0.011 02 |
| B_{1122} | 0.970 31 | 0.024 79 | 0.023 67 | 0.062 84 | 0.036 64 | 0.003 57 | 0.032 08 | 0.010 10 |
| B_{121} | 0.001 96 | 0.648 47 | 0.000 12 | 0.000 01 | 0.008 53 | 0.010 36 | 0.021 84 | 0.469 50 |
| B_{122} | 0.004 15 | 0.085 02 | 0.000 28 | 0.00 02 | 0.023 14 | 0.009 29 | 0.750 57 | 0.444 00 |
| B_2 | 0.001 77 | 0.028 81 | 0.000 76 | 0.000 90 | 0.000 06 | 0.965 52 | 0.007 26 | 0.036 16 |

| class | Na ₂ O | K ₂ O | CaO | MgO | Al ₂ O ₃ | Fe ₂ O ₃ ^a | SiO ₂ |
|------------|-------------------|------------------|----------|----------|--------------------------------|---|------------------|
| B_{111} | 0.274 88 | 0.944 82 | 0.004 32 | 0.610 29 | 0.014 39 | 0.760 21 | 0.028 08 |
| B_{1121} | 0.583 91 | 0.026 03 | 0.825 72 | 0.243 11 | 0.005 20 | 0.067 05 | 0.012 94 |
| B_{1122} | 0.139 83 | 0.013 00 | 0.167 67 | 0.142 34 | 0.004 69 | 0.048 65 | 0.012 55 |
| B_{121} | 0.000 22 | 0.004 67 | 0.000 35 | 0.001 13 | 0.902 10 | 0.030 08 | 0.048 24 |
| B_{122} | 0.000 50 | 0.011 27 | 0.000 79 | 0.002 60 | 0.037 56 | 0.093 75 | 0.039 48 |
| B_2 | 0.000 67 | 0.000 22 | 0.001 15 | 0.000 54 | 0.036 06 | 0.000 26 | 0.858 71 |

^a Denotes the chemical analysis of the aluminosilicates residue.**Table 4.** The Classic Partition Corresponding to the Final Fuzzy Muds Partition

| class | samples |
|------------|-------------------------|
| A_{111} | Krinides |
| A_{1121} | Lisbori |
| A_{1122} | Argilla Solare |
| A_{121} | Pikrolimni |
| A_{122} | Thermi, Kyllini, Boario |
| A_2 | Black mud |

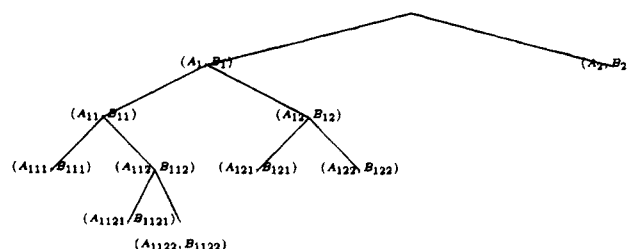
Table 5. The Classic Partition Corresponding to the Final Fuzzy Characteristics Partition

| class | samples |
|------------|---|
| B_{111} | organic, K ₂ O, MgO, Fe ₂ O ₃ ^a |
| B_{1121} | Na ⁺ , Cl ⁻ , SO ₄ ²⁻ , MgCO ₃ , Fe ₂ O ₃ , Na ₂ O, CaO |
| B_{1122} | K ⁺ , Ca ²⁺ , Mg ²⁺ , HCO ₃ ⁻ , NO ₃ ⁻ , CO ₃ ²⁻ |
| B_{121} | CaCO ₃ , CEC, Al ₂ O ₃ |
| B_{122} | pH |
| B_2 | ash, SiO ₂ |

^a Denotes the chemical analysis of the aluminosilicates residue.

final fuzzy characteristics partition. Tables 4 and 5 show the classical partitions corresponding to the two final fuzzy partitions obtained.

By a careful examination of the Tables 4 and 5, it is easy to notice that the "Black mud" sample is quite different with respect to all the others. This remarkable individuality is determined by a low content of ash and SiO₂. The low content of ash is strongly correlated to a relatively high content of HCO₃²⁻ and CO₃²⁻. In an opposite side appears the Krinides sample (set A_{111}). The singularity of this sample is due to high organic amount, a high content of K₂O, and

**Figure 1.** The classification hierarchy of the set of muds.

a low content of MgO and Fe₂O₃^(*). The position of Pikrolimni and thermi between Argilla Solare and Boario, within the partition tree, confirms the conclusion concerning their potential as beautifying muds. The position of the Lisbori sample is between Argilla Solare and Krinides, which appears to exhibit the poorest mud characteristics. Contrary to the conclusion of the authors of the cited paper, based on a subjective visual examination, the position of Kyllini indicates good mud characteristics, much closer to the best mud, Argilla Solare, Boario, and Black mud, respectively.

4. CONCLUDING REMARKS

The output of a fuzzy algorithm includes not only a partition but also additional information in the form of membership values. Moreover, the fuzzy cross-classification algorithm produces both a fuzzy objects partition and a fuzzy characteristics partition, "compatible" with the former. Thus, the advantages of this algorithm include the ability to observe not only the fuzzy classes obtained and the relations between them but also the characteristics corresponding to each final

class of objects (and which have contributed to the separation of the respective class).

Fuzzy cross-classification approach of muds based on their physico-chemical characteristics allows objective interpretation of their origin and maturation and helps in their classification. It also allows the quantitative and qualitative identification of the components influencing mud's physico-chemical properties and their therapeutical potential.

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