

## FCM: THE FUZZY $c$ -MEANS CLUSTERING ALGORITHM

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**Abstract**—This paper transmits a FORTRAN-IV coding of the fuzzy  $c$ -means (FCM) clustering program. The FCM program is applicable to a wide variety of geostatistical data analysis problems. This program generates fuzzy partitions and prototypes for any set of numerical data. These partitions are useful for corroborating known substructures or suggesting substructure in unexplored data. The clustering criterion used to aggregate subsets is a generalized least-squares objective function. Features of this program include a choice of three norms (Euclidean, Diagonal, or Mahalanobis), an adjustable weighting factor that essentially controls sensitivity to noise, acceptance of variable numbers of clusters, and outputs that include several measures of cluster validity.

**Key Words:** Cluster analysis, Cluster validity, Fuzzy clustering, Fuzzy QMODEL, Least-squared errors.

### INTRODUCTION

In general, cluster analysis refers to a broad spectrum of methods which try to subdivide a data set  $X$  into  $c$  subsets (clusters) which are pairwise disjoint, all nonempty, and reproduce  $X$  via union. The clusters then are termed a hard (i.e., nonfuzzy)  $c$ -partition of  $X$ . Many algorithms, each with its own mathematical clustering criterion for identifying "optimal" clusters, are discussed in the excellent monograph of Duda and Hart (1973). A significant fact about this type of algorithm is the defect in the underlying axiomatic model that each point in  $X$  is unequivocally grouped with other members of "its" cluster, and thus bears no apparent similarity to other members of  $X$ . One such manner to characterize an individual point's similarity to all the clusters was introduced in 1965 by Zadeh (1965). The key to Zadeh's idea is to represent the similarity a point shares with each cluster with a function (termed the membership function) whose values (called memberships) are between zero and one. Each sample will have a membership in every cluster, memberships close to unity signify a high degree of similarity between the sample and a cluster while memberships close to zero imply little similarity between the sample and that cluster. The history, philosophy, and derivation of such mathematical systems are documented in Bezdek (1981). The net effect of such a function for clustering is to produce fuzzy  $c$ -partitions of a given data set. A fuzzy  $c$ -partition of  $X$  is one which characterizes the membership of each sample point in all the clusters by a membership function which ranges between

zero and one. Additionally, the sum of the memberships for each sample point must be unity.

Let  $Y = \{y_1, y_2, \dots, y_N\}$  be a sample of  $N$  observations in  $\mathbb{R}^n$  ( $n$ -dimensional Euclidean space);  $y_k$  is the  $k$ -th feature vector;  $y_{kj}$  the  $j$ -th feature of  $y_k$ . If  $c$  is an integer,  $2 \leq c < n$ , a conventional (or "hard")  $c$ -partition of  $Y$  is a  $c$ -tuple  $(Y_1, Y_2, \dots, Y_c)$  of subsets of  $Y$  that satisfies three conditions:

$$Y_i \neq \phi \quad 1 \leq i \leq c; \quad (1a)$$

$$Y_i \cap Y_j = \phi; \quad i \neq j \quad (1b)$$

$$\bigcup_{i=1}^c Y_i = Y \quad (1c)$$

In these equations,  $\phi$  stands for the empty set, and  $(\cap, \cup)$  are respectively, intersection, and union.

In the context discussed later, the sets  $\{Y_i\}$  are termed "clusters in  $Y$ ". Clusters analysis (or simply clustering) in  $Y$  refers to the identification of a distinguished  $c$ -partition  $\{\hat{Y}_i\}$  of  $Y$  whose subsets contain points which have high intracluster resemblance; and, simultaneously, low intercluster similarity. The mathematical criterion of resemblance used to define an "optimal"  $c$ -partition is termed a cluster criterion. One hopes that the substructure of  $Y$  represented by  $\{\hat{Y}_i\}$  suggests a useful division or relationship between the population variables of the real physical process from whence  $Y$  was drawn. One of the first questions one might ask is whether  $Y$  was drawn. One of the first questions one might ask is whether  $Y$  contains any clusters at all. In many

geological analyses, a value for  $c$  is known *a priori* on physical grounds. If  $c$  is unknown, then determination of an optimal  $c$  becomes an important issue. This question is sometimes termed the "cluster validity" problem. Our discussion, in addition to the clustering *a posteriori* measures of cluster validity (or "goodness of fit").

Algorithms for clustering and cluster validity have proliferated due to their promise for sorting out complex interactions between variables in high dimensional data. Excellent surveys of many popular methods for conventional clustering using deterministic and statistical clustering criteria are available; for example, consult the books by Duda and Hart (1973), Tou and Gonzalez (1974), or Hartigan (1975). The conventional methodologies discussed in these references include factor analytic techniques, which occupy an important place in the analysis of geoscientific data. The principal algorithms in this last category are embodied in the works of Klovan and Imbrie (1971), Klovan and Miesch (1976), and Miesch (1976a, 1976b). These algorithms for the factor analytical analysis of geoscientific data are known as the QMODEL algorithms (Miesch, 1976a).

In several recent studies, the inadequacy of the QMODEL algorithms for linear unmixing when confronted with certain geometrical configurations in grain shape data has been established numerically (Full, Ehrlich, and Klovan, 1981; Full, Ehrlich, and Bezdek, 1982; Bezdek, and others, 1982). The problem is caused by the presence of outliers. Aberrant points may be real outliers, noise, or simply due to measurement errors; however, peculiarities of this type can cause difficulties for QMODEL that cannot be resolved by standard approaches. The existence of this dilemma led the authors to consider fuzzy clustering methods as an adjunct procedure which might circumvent the problems caused by data of this type. Because fuzzy clustering is most readily understood in terms of the axioms underlying its rationale, we next give a brief description of the basic ideas involved in this model.

### FUZZY CLUSTERING

The FCM algorithms are best described by recasting conditions (equation 1) in matrix-theoretic terms. Towards this end, let  $U$  be a real  $c \times N$  matrix,  $U = [u_{ik}]$ .  $U$  is the matrix representation of the partition  $\{Y_i\}$  in equation (1) in the situation

$$u_i(y_k) = u_{ik} = \begin{cases} 1; & y_k \in Y_i \\ 0; & \text{otherwise} \end{cases} \quad (2a)$$

$$\sum_{i=1}^N u_{ik} > 0 \quad \text{for all } i; \quad (2b)$$

$$\sum_{i=1}^N u_{ik} = 1 \quad \text{for all } k. \quad (2c)$$

In equation (2),  $u_i$  is a function;  $u_i: Y \rightarrow \{0, 1\}$ . In conventional models,  $u_i$  is the characteristic function of  $Y_i$ ; in fact,  $u_i$  and  $Y_i$  determine one another, so there is no harm in labelling  $u_i$  the  $i$ th hard subset of the partition (it is unusual, of course, but is important in terms of understanding the term "fuzzy set"). Conditions of equations (1) and (2) are equivalent, so  $U$  is termed a hard  $c$ -partition of  $Y$ . Generalizing this idea, we refer to  $U$  as a fuzzy  $c$ -partition of  $Y$  when the elements of  $U$  are numbers in the unit interval  $[0, 1]$  that continue to satisfy both equations (2b) and (2c). The basis for this definition are  $c$  functions  $u_i: Y \rightarrow [0, 1]$  whose values  $u_i(y_k) \in [0, 1]$  are interpreted as the grades of membership of the  $y_k$ s in the "fuzzy subsets"  $u_i$  of  $Y$ . This notion is due to Zadeh (1965), who conceived the idea of the fuzzy set as a means for modelling physical systems that exhibit nonstatistical uncertainties. Detailed discussions for the rationale and philosophy of fuzzy sets are available in many recent papers and books (e.g., consult Bezdek (1981)).

For the present discussion, it suffices to note that hard partitions of  $Y$  are a special type of fuzzy ones, wherein each data point is grouped unequivocally with its intracluster neighbors. This requirement is a particularly harsh one for physical systems that contain mixtures, or hybrids, along with pure or antecedent strains. Outliers (noise or otherwise) generally fall into the category one should like to reserve for "unclassifiable" points. Most conventional models have no natural mechanism for absorbing the effects of undistinctive or aberrant data, this is a direct consequence of equation (1a). Accordingly, the fuzzy set, and, in turn, fuzzy partition, were introduced as a means for altering the basic axioms underlying clustering and classification models with the aim of accommodating this need. By this device, a point  $y_k$  may belong entirely to a single cluster, but in general, is able to enjoy partial membership in several fuzzy clusters (e.g., precisely the situation anticipated for hybrids). We denote the sets of all hard and fuzzy  $c$ -partitions of  $Y$  by:

$$M_c = \{U_{c \times N} | u_{ik} \in [0, 1]; \text{ equations (2b), (2c)}\}; \quad (3a)$$

$$M_{fc} = \{U_{c \times N} | u_{ik} \in [0, 1]; \text{ equations (2b), (2c)}\}. \quad (3b)$$

Note that  $M_c$  is imbedded in  $M_{fc}$ . This means that fuzzy clustering algorithms can obtain hard  $c$ -partitions. On the other hand, hard clustering algorithms cannot determine fuzzy  $c$ -partitions of  $Y$ . In other words, the fuzzy imbedment enriches (not replaces!) the conventional partitioning model. Given that fuzzy  $c$ -partitions have at least intuitive appeal, how does one use the data to determine them? This is the next question we address.

Several clustering criteria have been proposed for identifying optimal fuzzy  $c$ -partitions in  $Y$ . Of these, the most popular and well studied method to date is

associated with the generalized least-squared errors functional

$$J_m(U, v) = \sum_{k=1}^N \sum_{i=1}^c (u_{ik})^m \|y_k - v_i\|_A^2 \quad (4)$$

Equation (4) contains a number of variables: these are

- $Y = \{y_1, y_2, \dots, y_N\} \subset \mathbf{R}^n =$  the data, (5a)
- $c =$  number of clusters in  $Y$ ;  $2 \leq c < n$ , (5b)
- $m =$  weighting exponent;  $1 \leq m < \infty$ , (5c)
- $U =$  fuzzy  $c$ -partition of  $Y$ ;  $U \in M_{fc}$  (5d)
- $v = (v_1, v_2, \dots, v_c) =$  vectors of centers, (5e)
- $v_i = (v_{i1}, v_{i2}, \dots, v_{in}) =$  center of cluster  $i$ , (5f)
- $\| \cdot \|_A =$  induced  $A$ -norm on  $\mathbf{R}^n$  (5g)
- $A =$  positive-definite ( $n \times n$ ) weight matrix. (5h)

The squared distance between  $y_k$  and  $v_i$  shown in equation (4) is computed in the  $A$ -norm as

$$d_{ik}^2 = \|y_k - v_i\|_A^2 = (y_k - v_i)^T A (y_k - v_i). \quad (6)$$

The weight attached to each squared error is  $(u_{ik})^m$ , the  $m$ th power of  $y_k$ 's membership in cluster  $i$ . The vectors  $\{v_i\}$  in equation (5f) are viewed as "cluster centers" or centers of mass of the partitioning subsets. If  $m = 1$ , it can be shown that  $J_m$  minimizes only at hard  $U$ 's  $\in M_c$ , and corresponding  $v_i$ 's are just the geometric centroids of the  $Y_i$ 's. With these observations, we can decompose  $J_m$  into its basic elements to see what property of the points  $\{y_k\}$  it measures:

- $d_{ik}^2 =$  squared  $A$ -distance from point  $y_k$  to center of mass  $v_i$ . (7a)
- $(u_{ik})^m d_{ik}^2 =$  squared  $A$ -error incurred by representing  $y_k$  by  $v_i$  weighted by (a power of) the membership of  $y_k$  in cluster  $i$ . (7b)
- $\sum_{i=1}^c (u_{ik})^m d_{ik}^2 =$  sum of squared  $A$ -errors due to  $y_k$ 's partial replacement by all  $c$  of the centers  $\{v_i\}$ . (7c)
- $\sum_{k=1}^N \sum_{i=1}^c (u_{ik})^m d_{ik}^2 =$  overall weighted sum of generalized  $A$ -errors due to replacing  $Y$  by  $v$ . (7d)

The role played by most of the variables exhibited in equation (5) is clear. Two of the parameters of  $J_m$ , however warrant further discussion, namely,  $m$  and  $A$ . Weighting exponent  $m$  controls the relative weights placed on each of the squared errors  $d_{ik}^2$ . As  $m \rightarrow 1$  from earlier discussion partitions that minimize  $J_m$  become increasingly hard (and, as mentioned before, at  $m = 1$ , are necessarily hard). Conversely, each entry of optimal  $\hat{U}$ 's for  $J_m$  approaches  $(1/c)$  as  $m \rightarrow \infty$ . Consequently, increasing  $m$  tends to degrade

(blur, defocus) membership towards the fuzziest state. Each choice for  $m$  defines, all other parameters being fixed, one FCM algorithm. No theoretical or computational evidence distinguishes an optimal  $m$ . The range of useful values seems to be  $[1, 30]$  or so. If a test set is available for the process under investigation, the best strategy for selecting  $m$  at present seems to be experimental. For most data,  $1.5 \leq m \leq 3.0$  gives good results.

The other parameter of  $J_m$  that deserves special mention is weight matrix  $A$ . This matrix controls the shape that optimal clusters assume in  $\mathbf{R}^n$ . Because every norm on  $\mathbf{R}^n$  is inner product induced via the formula

$$\langle x, y \rangle_A = x^T A y, \quad (8)$$

there are infinitely many  $A$ -norms available for use in equation (4). In practice, however, only a few of these norms enjoy widespread use. The FCM listing below allows a choice of three norms, each induced by a specific weight matrix. Let

$$c_y = \sum_{k=1}^N y_k |N|; \quad (9a)$$

$$C_y = \sum_{k=1}^N (y_k - c_y)(y_k - c_y)^t; \quad (9b)$$

be the sample mean and sample covariance matrix of data set  $Y$ ; and let  $\{a_i\}$  denote the eigenvalues of  $C_y$ ; let  $D_y$  be the diagonal matrix with diagonal elements  $(d_y)_{ii} = a_i$ ; and finally, let  $I$  be the identity matrix. The norms of greatest interest for use with equation (4) correspond to

$$A = I \sim \text{-Euclidean Norm,} \quad (10a)$$

$$A = D_y^{-1} \sim \text{Diagonal Norm,} \quad (10b)$$

$$A = C_y^{-1} \sim \text{Mahalonobis Norm.} \quad (10c)$$

A detailed discussion of the geometric and statistical implications of these choices can be seen in Bezdek (1981). When  $A = I$ ,  $J_m$  identifies hyperspherical clusters; for any other  $A$ , the clusters are essentially hyperellipsoidal, with axes proportional to the eigenvalues of  $A$ . When the diagonal norm is used, each dimension is effectively scaled via the eigenvalues. The Euclidean norm is the only choice for which extensive experience with geological data is available.

Optimal fuzzy clusterings of  $Y$  are defined as pairs  $(\hat{U}, \hat{v})$  that locally minimize  $J_m$ . The necessary conditions for  $m = 1$  are well known (but hard to use, because  $M_c$  is discrete, but large). For  $m > 1$ , if  $y_k \neq \hat{v}_j$  for all  $j$  and  $k$ ,  $(\hat{U}, \hat{v})$  may be locally optimal for  $J_m$  only if

$$\hat{v}_i = \sum_{k=1}^N (\hat{u}_{ik})^m y_k / \sum_{k=1}^N (\hat{u}_{ik})^m; \quad 1 \leq i \leq c; \quad (11a)$$

$$\hat{u}_{ik} = \left( \sum_{j=1}^c \left( \frac{\hat{d}_{ik}}{\hat{d}_{jk}} \right)^{2/(m-1)} \right)^{-1}; \quad 1 \leq k \leq N; 1 \leq i \leq c \quad (11b)$$

where  $\hat{d}_{ik} = \|y_k - \hat{v}_i\|_A$ . Conditions expressed in equations (11) are necessary, but not sufficient; they provide means for optimizing  $J_m$  via simple Picard iteration, by looping back and forth from equation (11a) to (11b) until the iterate sequence shows but small changes in successive entries of  $\hat{U}$  or  $\hat{v}$ . We formalize the general procedure as follows:

*Fuzzy c-Means (FCM) Algorithms*

- (A1) Fix  $c, m, A, \|k\|_A$ . Choose an initial matrix  $U^{(0)} \in M_{fc}$ . Then at step  $k, k = 0, 1, \dots, LMAX$ .
- (A2) Compute means  $\hat{v}^{(k)}, i = 1, 2, \dots, c$  with equation (11)a.
- (A3) Compute an updated membership matrix  $\hat{U}^{(k+1)} = [\hat{u}_{ik}^{(k+1)}]$  with equation (11b).
- (A4) Compare  $\hat{U}^{k+1}$  to  $\hat{U}^{(k)}$  in any convenient matrix norm. If  $\|\hat{U}^{(k+1)} - \hat{U}^{(k)}\| < \epsilon$ , stop. Otherwise, set  $\hat{U}^{(k)} = \hat{U}^{k+1}$  and return to (A2).

(A1)–(A4) is the basic algorithmic strategy for the FCM algorithms.

Individual control parameters, tie-breaking rules, and computing protocols are discussed in conjunction with the appended FORTRAN listing in Appendix 1.

Theoretical convergence of the sequence  $\{\hat{U}^{(k)}, \hat{v}^{(k)}, k = 0, 1, \dots\}$  generated by (A1)–(A4) has been studied (by Bezdek, 1981). Practically speaking, no difficulties have ever been encountered, and numerical convergence is usually achieved in 10–25 iterations. Whether local minima of  $J_m$  are good clusterings of  $Y$  is another matter, for it is easy to obtain data sets upon which  $J_m$  minimizes globally with visually unappealing substructure. To mitigate this difficulty, several types of cluster validity functionals are usually calculated on each  $\hat{U}$  produced by FCM. Among the most popular are the partition coefficient and entropy of  $\hat{U} \in M_{fc}$ :

$$F_c(\hat{U}) = \sum_{k=1}^N \sum_{i=1}^c (\hat{u}_{ik})^2 / N; \tag{12a}$$

$$H_c(\hat{U}) = - \sum_{k=1}^N \sum_{i=1}^c (\hat{u}_{ik} \log_a(\hat{u}_{ik})) / N. \tag{12b}$$

In equation (12b), logarithmic base  $a \in (1, \infty)$ . Properties of  $F_c$  and  $H_c$  utilized for validity checks are:

$$F_c = 1 \Leftrightarrow H_c = 0 \Leftrightarrow \hat{U} \in M_c \text{ is hard}; \tag{13a}$$

$$F_c = 1/c \Leftrightarrow H_c = \log_a(c) \Leftrightarrow \hat{U} = [1/c]; \tag{13b}$$

$$\frac{1}{c} \leq F_c \leq 1; \quad 0 \leq H_c \leq \log_a(c). \tag{13c}$$

Entropy  $H$  is a bit more sensitive than  $F$  to local changes in partition quality. The FCM program listed below calculates  $F, H$ , and  $(1 - F)$ , the latter quantity owing to the inequality  $(1 - F) < H$  for  $\hat{U} \notin M_c$  (when  $a = e = 2.71 \dots$ ).

Finally, we observe that generalizations of  $J_m$  which can accommodate a much wider variety of data shapes than FCM are now well known (see Bezdek (1981) for a detailed account). Nonetheless, the basic FCM algorithm remains one of the most useful general purpose fuzzy clustering routines, and is the one utilized in the FUZZY QMODEL algorithms discussed by Full, Ehrlich, and Bezdek (1982). Having given a brief account of the generalities, we now turn to computing protocols for the FCM listing accompanying this paper.

**ALGORITHMIC PROTOCOLS**

The listing of FCM appended below has some features not detailed in (A1)–(A4). Our description of the listing corresponds to the blocks as documented.

*Input Variables.* FCM arrays are listing documented. Symbolic dimensions are

NS = number of vectors in  $Y = N$ .

ND = number of features in  $y_k = n$ .

Present dimensions will accommodate up to  $c = 20$  clusters,  $N = 500$  data points, and  $n = 20$  features. Input variables ICON specifies the weight matrix  $A$  as in equation (10):

$$\text{ICON} = 1 \Rightarrow A = I$$

$$\text{ICON} = 2 \Rightarrow A = D_y^{-1}.$$

$$\text{ICON} = 3 \Rightarrow A = C_y^{-1}.$$

Other parameters read are:

QQ = Weighting exponent  $m: 1 < QQ$ .

KBEGIN = Initial number of clusters:

$$2 \leq \text{KBEGIN} \leq \text{DCEASE}.$$

KCEASE = Final number of clusters:

$$\text{KCEASE} < \text{NS}.$$

At any step  $\text{NCLUS} = C$  is the operating number of clusters. FCM iterates over NCLUS from KBEGIN to KCEASE, generating an optimal pair  $(\hat{U}, \hat{v})_{\text{NCLUS}}$  for each number of clusters desired. Changes in  $m$  and  $A$  must be made between runs (although they could easily be made iterate parameters).

*Control Parameters*

EPS = Termination criterion  $\epsilon$  in (A4).

LMAX = Maximum number iterations at each  $c$  in (A1).

Current values of EPS and LMAX are 0.01 and 50. Lowering EPS almost always results in more iterations to termination.

**Input *Y***

*Compute Feature Means.* Vector FM(ND) is the mean vector  $c_j$  of equation (9a).

*Compute Scaling Matrix.* Matrix CC(ND, ND) is matrix *A* of equation (10), depending upon the choice made for ICON. The inverse is constructed in the main to avoid dependence upon peripheral subs. Matrix CM =  $A^*A^{-1}$  calculated as a check on the computed inverse, but no residual is calculated; nor does the FCM routine contain a flag if CM is not "close" to *I*. The construction of weight matrices other than the three choices allowed depends on user definition.

*Loop Control.* NCLUS = *c* is the current number of clusters: QQ is the weighting exponent *m*.

*Initial Guess.* A pseudo-random initial guess for  $U_0$  is generated in this block at each access.

*Cluster Centers.* Calculation of current centers V(NC, ND) via equation (11a).

*Update Memberships.* Calculations with equation (11b); W(NC, ND) is the updated membership matrix. The special situation  $m = 1$  is not accounted for here. Many programs are available for this situation for example see Ball (1965). The authors will furnish a listing for hard *c*-means upon request. Note that this block does not have a transfer in situation  $y_k = \hat{v}_i$  for some *k* and *i*. This eventuality to our knowledge, has never occurred in nearly 10 years of computing experience. If a check and assignment are desired, the method for assigning  $\hat{u}'_i$ s in any column *k* where such a singularity occurs is arbitrary, as long as constraints in equation (2) are satisfied. For example, one may, in this instance, place equal weights (that sum to one) on every row where  $y_k = \hat{v}_i$ , and zero weights otherwise. This will continue the algorithm, and roundoff error alone should carry the sequence away from such points.

*Error Criteria and Cutoffs.* The criterion used to terminate iteration at fixed NC is

$$ERRMAX = \max_{i,k} \{ |\hat{u}_{ik}^{(k+1)} - \hat{u}_{ik}^{(k)}| \} < EPS. \quad (14)$$

Threshold EPS thus controls the accuracy of terminal output. An alternative method to terminate iteration would be to compare components of each  $\hat{v}_i^{(k+1)}$  to  $\hat{v}_i^{(k)}$ . There may be differences in terminal pairs ( $\hat{U}, \hat{v}$ ) obtained using a fixed EPS. Furthermore, there is a tradeoff in CPU time, equation (14) requires (*cN*) comparisons and  $\max_{ij} \{ |\hat{v}_{ij}^{(k+1)} - \hat{v}_{ij}^{(k)}| \}$  requires (*cn*)

comparisons. Thus, if *N* is much larger than *n*, ( $N \gg n$ ), termination based on the quality of successive cluster centers computed via equation (11a) becomes more attractive. By the same token, this can reduce storage space (for updated centers instead of an updated membership matrix) significantly if  $n \ll N$ . If equation (14) is never satisfied, iteration at current NC will stop when  $k = LMAX$ : a convergence flag is issued, and NC advance to NC + 1. More than 25 iterations are rarely needed for EPS in the 0.001 range.

*Cluster Validity Indicators.* Values of  $J_m, F_c, H_c,$  and  $1 - F_c$  are computed, and stored, respectively, in the vectors *VJM, F, H,* and *DIF*.

*Output Block.* For the current value of NCLUS, current terminal values of  $F_c, 1 - F_c, H_c, J_m, \{\hat{v}_{ij}\},$  and  $\hat{U}$  are printed.

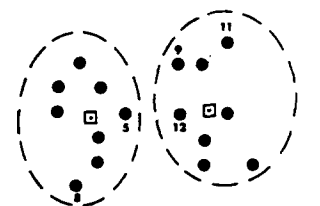
*Output Summary.* The final block of FCM outputs statistics for the entire run.

The listing provided is a very basic version of FCM: many embellishments are discussed in Bezdek (1981). As an aid for debugging a coded copy of the listing, we present a short example that furnishes a means for checking numerical outputs. This example highlights several of the important features of fuzzy *z*-partitions in general, and those generated by FCM in particular. Examples of the use of FCM in the context of geological data analysis are presented in Bezdek, and other (1982), and Full, Ehrlich, and Bezdek (1982).

*Storage Requirements.* The program listed in the appendix can handle 500 data samples with up to 50 variables. It will handle up to 20 clusters. The program, as written, used under 256 K of computer storage. If larger data sets are used, the program is clearly documented as to which parameters to change.

**A NUMERICAL EXAMPLE**

Figure 1 displays a set *Y* of 16 points in  $R^2$ . This artificial data set was originally published in Sneath



No.	Coordinates	
	$y_{k1}$	$y_{k2}$
1	0	4
2	0	3
3	1	5
4	2	4
5	3	3
6	2	2
7	2	1
8	1	0
9	5	5
10	6	5
11	7	6
12	5	3
13	7	3
14	6	2
15	6	1
16	8	1

□ = Terminal cluster centers from Table 2, col. 3

⋮ = Terminal maximum membership "boundaries".

Fig. 1. An example: Artificial touching clusters.

and Sokal (1973) in connection with the illustration of a hard clustering algorithm called the unpaired group mean average (UPGMA) method. This data was subsequently studied in Bezdek (1974), where a comparison between the UPGMA and FCM methods was effected. The coordinates of  $y_k \in Y$  are listed as columns two and three of the tabular display of Fig. 1. This is a good data set for our purposes because it is easily handled for validation, and further, has some of the geometric properties that necessitate the introduction of fuzzy models. Data of this type might be drawn from a mixture of two bivariate normal distributions. The region of overlap contains several points which might be considered "noise", viz.  $y_5$  and  $y_{12}$ . Parameters for the outputs to be discussed were as follows:

Table	ICON = A	NCLUS = c	QQ = m	EPS = $\epsilon$
1	1, 2, 3	2	2	0.01
2	2	2	1.25, 2.00	0.01
3	1	2-6	1.25-2.00	0.01

In other words, we illustrate in Tables 1 and 2, respectively, the effects of variation in the norm inducing matrix  $A$ , and weighting exponent on  $(\hat{U}, \hat{v})$  with all other parameters being fixed; while Table 3 exhibits variations in  $F_c$  and  $H_c$  due to changes in  $m$  and  $c$ .

Initial guesses for  $U_0$  were not chosen randomly here, so that users may validate their programs against

these tables. Rather, the initial matrix used for all of the outputs discussed later had the following elements:

$$(U_0)_{ii} = \left(\frac{\alpha}{c} + \beta\right); \quad i = 1, 2, \dots, c$$

$$(U_0)_{ij} = \left(\frac{\alpha}{c} + \beta\right); \quad j = c + 1, \dots, n$$

$$(U_0)_{ij} = \left(\frac{\alpha}{c} + \beta\right); \quad \text{otherwise}$$

$$\alpha = 1 - (\sqrt{2}/2);$$

$$\beta = \sqrt{2}/2.$$

The starting value for  $F_c$  using this  $U_0$  is always the midpoint of  $[1/c, 1)$ , the range of  $F_c$ , that is  $f_c(U_0) = ((1/c) + 1)/2$ . In real applications it is, of course, important to run FCM for several different  $U_0$ s, as the iteration method used, like all descent methods, is susceptible to local stagnations. If different  $U_0$ s result in different  $(\hat{U}, \hat{v})$ s, one thing is certain: further analysis should be made before one places much confidence in any algorithmically suggested substructure in  $Y$ .

Table 1 shows that maximizing  $F_c$  is equivalent to minimizing  $H_c$  but this behavior is not equivalent to minimizing  $J_m$ . Several examples of the general dilemma are documented in Bezdek (1981). Observe that all three partitions of  $Y$  are (qualitatively) more or less equivalent. Lower membership generally cor-

Table 1. Variation in  $(\hat{U}, \hat{v})$  due to changes in Norm. There are only two clusters, hence  $\hat{U}_{2k} = (1 - \hat{U}_{1k})$  as the sum of the  $\hat{u}_{ik}$  equals one. Terminal membership  $U_{ik}$

Data Point	ICON = 1 A = I	ICON = 2 A = $D_y^{-1}$	ICON = 3 A = $C_y^{-1}$
1	0.92	0.88	0.89
2	0.95	0.93	0.92
3	0.86	0.78	0.82
4	0.91	0.88	0.93
5	0.80	0.84	0.84
6	0.95	0.88	0.82
7	0.86	0.72	0.55
8	0.82	0.67	0.62
9	0.22	0.35	0.43
10	0.12	0.26	0.33
11	0.18	0.32	0.37
12	0.10	0.08	0.09
13	0.02	0.03	0.04
14	0.06	0.09	0.06
15	0.16	0.24	0.19
16	0.15	0.21	0.19
$\hat{v}_{11}$	6.18	5.99	5.96
$\hat{v}_{12}$	3.15	2.95	2.75
$\hat{v}_{21}$	1.44	1.67	1.73
$\hat{v}_{22}$	2.83	3.01	3.19
$F_c$	0.80	0.71	0.71
$H_c$	0.35	0.45	0.45
$J_m$	51.65	13.69	13.69
Iter.	6	6	12

Table 2. Variation in  $(\hat{u}, \hat{v})$  due to changes in  $m$  (two cluster example). Terminal membership  $\hat{u}_{ik}: \hat{u}_{2k} = (1 - \hat{u}_{1k})$

Data Point	QQ = m = 1.25	QQ = m = 2.00
1	1.00	0.92
2	1.00	0.95
3	1.00	0.86
4	1.00	0.91
5	1.00	0.80
6	1.00	0.95
7	1.00	0.86
8	1.00	0.82
9	0.00	0.22
10	0.00	0.12
11	0.00	0.18
12	0.00	0.10
13	0.00	0.02
14	0.00	0.06
15	0.00	0.16
16	0.00	0.15
$\hat{v}_{11}$	6.25	6.18
$\hat{v}_{12}$	3.25	3.15
$\hat{v}_{21}$	1.37	1.44
$\hat{v}_{22}$	2.75	2.83
$F_c$	1.00	0.80
$H_c$	0.00	0.35
$J_m$	60.35	51.65
Iter.	4	6

Table 3. Variation in  $F$  and  $H$  due to changes in  $m$  and  $c$ .

Weighting Exponent (m)	Number of Clusters (c)	Partition Coefficient ( $F_c$ )	Lower Bound ( $1-F_c$ )	Normalized Entropy ( $H_c$ )
1.25	2	0.998	0.002	0.007
	3	0.983	0.017	0.037
	4	0.979	0.021	0.044
	5	0.996	0.004	0.013
1.50	2	0.955	0.045	0.103
	3	0.903	0.097	0.202
	4	0.901	0.099	0.201
	5	0.917	0.083	0.197
1.75	2	0.873	0.127	0.239
	3	0.791	0.209	0.404
	4	0.804	0.196	0.401
	5	0.776	0.224	0.468
2.00	2	0.794	0.206	0.352
	3	0.686	0.314	0.575
	4	0.700	0.300	0.600
	5	0.662	0.338	0.701

responds to points distant from the "core" (i.e.  $\hat{v}_i$ ) of cluster  $i$ . Thus, point 8 is clearly signaled an outlier, for example in all three partitions. Notice, however, that the Mahalanobis norm emphasizes this much more heavily than, for example the Euclidean norm. This is because level sets in the former norm are elliptical, and in the latter circular. Thus, the variance of  $y_8$  in the vertical direction weights its influence

differently. In all situations, points near cluster centers in the  $A$ -norm have higher memberships. Note that  $\hat{v}_1$  is more stable to changes in  $A$  than  $v_2$ : this indicates that points with a high affinity for membership in  $\hat{u}_2$  have somewhat more variability than those seeking to associate with  $\hat{u}_1$ . Table 1 also demonstrates another general fact; the number of iterates needed using the Mahalanobis norm is usually higher than

the number required by other norms. See Bezdek (1981) for more discussion concerning characteristic cluster shapes associated with changes in  $A$ .

Table 2 illustrates the usual effect of increasing  $m$  lower  $m$ 's yield harder partitions and higher ones, fuzzier memberships. For  $m = 1.25$ ,  $\hat{U}$  is hard (to 2 decimal places). Observe that  $F_c$  and  $H_c$  mirror this fact, but again,  $J_m$  does not, having a higher value at the lower  $m$ . Further observe that the cluster centers are rather stable to changes in  $m$ . This is not always the situation, and it is an unproven conjecture that the stability of the  $\hat{v}_i$ 's in the face of severe changes in  $m$  is in some sense an indication of cluster validity. Figure 1 exhibits  $\hat{v}_1$  and  $\hat{v}_2$  for  $m = 2 = c$ ,  $A = I$ ; their geometric positions are at least (visually) appealing.

Table 3 depicts the utility of  $F_c$  and  $H_c$  for the cluster validity question. For every  $m$ ,  $F_c$  maximizes (and  $H_c$  minimizes) at  $c = 2$ . From this we can infer that the "hardest" substructure detectable in  $Y$  occurs are  $c = 2$ . These values do not, however, have any direct tie to  $Y$ . Being computed on algorithmic outputs based on  $Y$  rather than any concrete assumptions regarding the distribution of  $Y$  somewhat weakens the theoretical plausibility of using  $F_c$  and  $H_c$  for cluster validity. Nevertheless, they have been demonstrably reliable in many experimental studies, and are, at present, the most reliable indicants of validity for the FCM algorithms.

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#### APPENDIX

##### Listing of fuzzy C-means

FILE: KMEANS FORTRAN A 03/18/83 11:05 VM/SP CONVERSATIONAL MONITOR SYSTEM

```

C
C
C THIS IS THE FCM (FUZZY C-MEANS) ROUTINE. THIS LISTING IS FOR A
C IBM TYPE COMPUTER WITH A FORTRAN IV COMPILER. IT ADAPTS FOR ANY
C FORTRAN COMPILER WITH MODIFICATIONS SET AT THE USER SITE.
C
C REFERENCE: "PATTERN RECOGNITION WITH FUZZY OBJECTIVE FUNCTIONS,"
C JAMES BEZDEK, PLENUM, NEW YORK, 1981.
C
C DESCRIPTION OF OPERATING VARIABLES:
C I. INPUT VARIABLES (FROM FILE 5)
C CARD 1:
C TITLE(20).....80 CHARACTER HEADING
C CARD 2:
C FMT(20).....FORTRAN FORMAT (CONTAINED IN PARENTHESIS)
C DESCRIBING THE INPUT FORMAT FOR THE RAW DATA
C UP TO 80 CHARACTERS MAY BE USED
C CARD 3:
C COL 1: ICON.....DISTANCE MEASURE TO BE USED. IF:
C ICON=1 USE EUCLIDEAN NORM
C ICON=2 USE DIAGONAL NORM
C ICON=3 USE MAHALANOBIS NORM
C COLS 2-7: QQ.....WEIGHTING EXPONENT FOR FCM
C COLS 8-9: ND.....NUMBER OF FEATURES PER INPUT VECTOR

```





```

DO 350 I=1,NDIM                                00100000
FM(I)=0.                                        00101000
DO 351 J=1,NSAMP                                00102000
351 FM(I)=FM(I)+Y(J,I)                          00103000
350 FM(I)=FM(I)/ANSAMP                          00104000
C-----
C FEATURE VARIANCES.                            00106000
C-----
DO 352 I=1,NDIM                                00108000
FVAR(I)=0.                                       00109000
DO 353 J=1,NSAMP                                00110000

```

FILE: KMEANS FCRTRAN A 03/18/83 11:05 VM/SP CONVERSATIONAL MONITOR SYSTEM

```

353 FVAR(I)=FVAR(I)+((Y(J,I)-FM(I))**2)         00111000
352 FVAR(I)=FVAR(I)/ANSAMP                       00112000
IF (ICON-1)380,38C,382                           00113000
380 DO 381 I=1,NDIM                              00114000
DO 381 J=1,NDIM                                  00115000
381 CC(I,J)=0.                                    00116000
DO 370 I=1,NDIM                                  00117000
370 CC(I,I)=1.                                    00118000
GO TO 390                                         00119000
382 IF (ICON-2)384,384,386                         00120000
384 DO 385 I=1,NDIM                              00121000
DO 385 J=1,NDIM                                  00122000
385 CC(I,J)=0.                                    00123000
DO 371 I=1,NDIM                                  00124000
371 CC(I,I)=1./FM(I)                             00125000
GO TO 390                                         00126000
386 DO 360 I=1,NDIM                              00127000
DO 360 J=1,NDIM                                  00128000
AA(I,J)=0.                                        00129000
DO 361 K=1,NSAMP                                  00130000
361 AA(I,J)=AA(I,J)+((Y(K,I)-FM(I))*(Y(K,J)-FM(J))) 00131000
360 AA(I,J)=AA(I,J)/ANSAMP                       00132000
DO 550 I=1,NDIM                                  00133000
DO 550 J=1,NDIM                                  00134000
550 ST(I,J)=AA(I,J)                              00135000
C-----
C INVERSION OF COVARIANCE MATRIX AA TO AI        00137000
C-----
NN=NDIM-1                                        00139000
AA(1,1)=1./AA(1,1)                              00140000
DO 500 M=1,NN                                     00141000
K=M+1                                             00142000
DO 501 I=1,M                                     00143000
BB(I)=0.                                          00144000
DO 501 J=1,M                                     00145000
501 BB(I)=BB(I)+AA(I,J)*AA(J,K)                 00146000
D=0.                                              00147000
DO 502 I=1,M                                     00148000
502 D=D+AA(K,I)*BB(I)                           00149000
D=-D+AA(K,K)                                    00150000
AA(K,K)=1./D                                     00151000
DO 503 I=1,M                                     00152000
503 AA(I,K)=-BB(I)*AA(K,K)                      00153000
DO 504 J=1,M                                     00154000
CCC(J)=0.                                        00155000
DO 504 I=1,M                                     00156000
504 CCC(J)=CCC(J)+AA(K,I)*AA(I,J)               00157000
DO 505 J=1,M                                     00158000
505 AA(K,J)=-CCC(J)*AA(K,K)                     00159000
DO 500 I=1,M                                     00160000
DO 500 J=1,M                                     00161000
500 AA(I,J)=AA(I,J)-BB(I)*AA(K,J)               00162000
DO 520 I=1,NDIM                                  00163000
DO 520 J=1,NDIM                                  00164000
520 AI(I,J)=AA(I,J)                             00165000

```

FILE: KMEANS FCRTRAN A 03/18/83 11:05 VM/SP CONVERSATIONAL MONITOR SYSTEM

```

DO 387 I=1,NDIM                                00166000
DO 387 J=1,NDIM                                00167000

```

```

387  CC(I,J)=AI(I,J)                                00168000
C-----00169000
C   CHECK INVERSE AA*AI=I                          00170000
C-----00171000
      DO 530 I=1,NDIM                                00172000
      DO 530 J=1,NDIM                                00173000
      CM(I,J)=0.                                     00174000
      DO 530 K=1,NDIM                                00175000
530  CM(I,J)=CM(I,J)+ST(I,K)*AI(K,J)               00176000
      WRITE(6,531)                                    00177000
531  FORMAT(' ',//,' CHECK MATRIX AI*AA=1, THE IDENTITY'//) 00178000
      DO 532 I=1,NDIM                                00179000
532  WRITE (6,533) (CM(I,J),J=1,NDIM)               00180000
533  FORMAT(10X,20F6.2)                              00181000
390  WRITE(6,1460) (TITLE(III),III=1,20)            00182000
1460 FORMAT('1',10X,20A4'//)                         00183000
      WRITE(6,420)                                    00184000
420  FORMAT(' ',//,15X,' SCALING MATRIX CC',//)      00185000
      DO 421 I=1,NDIM                                00186000
421  WRITE(6,422) (CC(I,J),J=1,NDIM)                00187000
422  FORMAT(5X,10(F10.1,1X)/5X,1C(F10.1,1X)/)       00188000
      WRITE(6,425)                                    00189000
425  FORMAT(/////)                                  00190000
C-----00191000
C   QQ IS THE BASIC EXPONENT FOR FUZZY ISGDATA.     00192000
C-----00193000
      PP=(1./(QQ-1.))                                 00194000
      DO 55555 NCLUS=KBEGIN,KCEASE                   00195000
      WRITE(6,1460) (TITLE(III),III=1,20)            00196000
      WRITE(6,499) NCLUS,ICCN,QQ                     00197000
499  FORMAT(' ', ' NUMBER OF CLUSTERS = ',I3,5X,' ICCN = ',I3,5X,
C'EXPONENT = ',F4.2,//)                             00198000
      IT=1                                           00199000
C-----00200000
C   RANDOM INITIAL GUESS FOR U(I,J)                 00201000
C   THE RANDOM GENERATOR SUBROUTINE RANDU FROM THE  00202000
C   SUBROUTINE PACKAGE (SSP) IS USED AND IS CALLED  00203000
C   FROM AN EXTERNAL LIBRARY. OTHER GENERATORS     00204000
C   THAT PRODUCE VALUES ON THE INTERVAL           00205000
C   ZERO TO ONE CAN BE USED.                        00206000
C-----00207000
      RANDOM=.7731                                    00208000
      IX=1                                             00209000
      NCLUS1=NCLUS-1                                  00210000
      DO 1100 K=1,NSAMP                               00211000
      S=1.0                                           00212000
      DO 1101 I=1,NCLUS1                              00213000
C   CALL RANDU(IX,IY,RANDOM)                          00214000
      RANDOM=RANDOM/2.                                00215000
      IX=IY                                           00216000
      ANC=NCLUS-I                                     00217000
      U(I,K)=S*(1.0-RANDOM**(1.0/ANC))                00218000
1101  S=S-U(I,K)                                     00219000
1100  U(NCLUS,K)=S                                   00220000

```

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```

C-----00221000
C   CALCULATION OF CLUSTER CENTERS V(I).            00222000
C-----00223000
7000 DO 20 I=1,NCLUS                                 00224000
      DO 20 J=1,NDIM                                 00225000
      V(I,J)=0.                                     00226000
      D=0.                                           00227000
      DO 21 L=1,NSAMP                               00228000
      V(I,J)=V(I,J)+((U(I,L)**QQ)*Y(L,J))           00229000
21  D=D+(U(I,L)**QQ)                                00230000
20  V(I,J)=V(I,J)/D                                 00231000
C-----00232000
C   UPDATE MEMBERSHIP FUNCTIONS.                    00233000
C-----00234000
6111 DO 38 I=1,NCLUS                                 00235000
      DO 38 J=1,NSAMP                               00236000
      W(I,J)=0.                                     00237000
      A=0.                                           00238000
      DO 31 L=1,NDIM                                00239000
      DO 31 M=1,NDIM                                00240000

```

```

31  A=A+((Y(J,L)-V(I,L))*CC(L,M)*(Y(J,M)-V(I,M)))          00241000
    A=1./(A**PP)                                           00242000
    SUM=0.                                                  00243000
    DO 32 N=1,NCLUS                                       00244000
    C=0.                                                    00245000
    DO 33 L=1,NDIM                                         00246000
    DO 33 M=1,NDIM                                         00247000
33  C=C+((Y(J,L)-V(N,L))*CC(L,M)*(Y(J,M)-V(N,M)))        00248000
    C=1./(C**PP)                                           00249000
32  SUM=SUM+C                                              00250000
    W(I,J)=A/SUM                                           00251000
38  CONTINUE                                              00252000
-----00253000
C   ERROR CRITERIA AND CUTOFFS.                            00254000
C   -----00255000
9000 ERRMAX=0.                                             00256000
    DO 40 I=1,NCLUS                                       00257000
    DO 40 J=1,NSAMP                                       00258000
    ERR=ABS(U(I,J)-W(I,J))                                00259000
    IF(ERR.GT.ERRMAX) ERRMAX=ERR                          00260000
40  CONTINUE                                              00261000
    WRITE(6,400) IT,ERRMAX,NCLUS                           00262000
400  FORMAT(1H,'ITERATION = ',I4,5X,'MAXIMUM ERROR = ',F10.4,
    110X,'NUMBER OF CLUSTERS = ',I4)                       00263000
    DO 42 I=1,NCLUS                                       00265000
    DO 42 J=1,NSAMP                                       00266000
42  U(I,J)=W(I,J)                                         00267000
    IF(ERRMAX.LE.EPS) GO TO 600C                          00268000
43  IT=IT+1                                               00269000
    IF(IT-LMAX) 7C00,7000,6000                            00270000
-----00271000
C   CALCULATION OF CLUSTER VALIDITY STATISTICS F, H, 1-E  00272000
C   -----00273000
6000 ITT(NCLUS)=IT                                        00274000
    F(NCLUS)=0.0                                          00275000

```

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```

    H(NCLUS)=0.0                                           00276000
    DO 100 I=1,NCLUS                                       00277000
    DO 100 K=1,NSAMP                                       00278000
    AU=U(I,K)                                              00279000
    F(NCLUS)=F(NCLUS)+AU**2/ANSAMP                        00280000
    IF (AU) 10G,100,101                                   00281000
101  H(NCLUS)=H(NCLUS)-AU*ALOG(AU)/ANSAMP                00282000
100  CONTINUE                                             00283000
    DIF(NCLUS)=1.0-F(NCLUS)                              00284000
-----00285000
C   CALCULATION OF OBJECTIVE FUNCTION                    00286000
C   -----00287000
    A=0.                                                  00288000
    DO 80 I=1,NCLUS                                       00289000
    DO 80 J=1,NSAMP                                       00290000
    DIST=0.                                               00291000
    DO 81 L=1,NDIM                                         00292000
    DO 81 M=1,NDIM                                         00293000
81  DIST=DIST+((Y(J,L)-V(I,L))*CC(L,M)*(Y(J,M)-V(I,M))) 00294000
    A=A+((U(I,J)**QQ)*DIST)                              00295000
80  VJM(NCLUS)=A                                         00296000
-----00297000
C   OUTPUT BLOCK FOR CURRENT NCLUS                      00298000
C   -----00299000
    WRITE(6,401)                                          00300000
401  FORMAT(' '///' FSTOP',7X,'1-FSTOP',5X,'ENTROPY',5X,'PAYOFF',5X,/) 00301000
    WRITE(6,699) F(NCLUS),DIF(NCLUS),H(NCLUS),VJM(NCLUS) 00302000
699  FORMAT(1H,2(F6.3,4X),4X,F6.3,5X,E8.3)              00303000
    WRITE(6,59)                                           00304000
59  FORMAT(1X,100('-')//)                                 00305000
    WRITE(6,402)                                          00306000
402  FORMAT(///,15X,'CLUSTER CENTERS V(I,J)',///).      00307000
    DO 415 I=1,NCLUS                                       00308000
415  WRITE(6,404) (I,J,V(I,J),J=1,NDIM)                 00309000
404  FORMAT(' I=',I3,3X,' J=',I3,3X,' V(I,J)=' ,F8.4)  00310000
405  FORMAT(1H,7(F6.4,3X))                               00311000
    WRITE(6,59)                                           00312000
    WRITE(6,406)                                          00313000

```

