# 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 Mahalonobis), 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  $Y = \{y_1, y_2, \ldots, y_N\}$  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,  $2 \le c < n$ , a conventional (or "hard") c-partition of Y is a c-tuple  $(Y_1, Y_2, \ldots, Y_c)$  of subsets of Y that satisfies three conditions:

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

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

$$\bigcup_{i=1}^{c} Y_i = Y \tag{1c}$$

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

In the context discussed later, the sets  $\{Y_1\}$  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-partion 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 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 OMODEL 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

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

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

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

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 cfunctions  $u_i$ :  $Y \rightarrow [0, 1]$  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 accompositing this need. By this device, a point  $v_k$ 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 cpartitions of Y by:

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

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

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

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

$$Y = \{y_1, y_2, \dots, y_N\} \subset \mathbf{R}^n = \text{the data}, \tag{5a}$$

$$c = \text{number of clusters in } Y; \quad 2 \le c < n,$$
 (5b)

$$m = \text{weighting exponent}; \quad 1 \le m < \infty,$$
 (5c)

$$U = \text{fuzzy } c\text{-partition of } Y; \quad U \in M_{fc}$$
 (5d)

$$v = (v_1, v_2, \dots, v_c) = \text{vectors of centers},$$
 (5e)

$$v_i = (v_{i1}, v_{i2}, \dots, v_{in}) = \text{center of cluster } i, \quad (5f)$$

$$\| \|_{A} = \text{induced } A \text{-norm on } \mathbb{R}^{n}$$
 (5g)

$$A = \text{positive-definite } (n \times n) \text{ weight matrix.}$$
 (5h)

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

$$d_{ik}^2 = \|y_k - v_i\|_A^2 = (y_k - v_1)^T A(y_k - v_i).$$
 (6)

The weight attached to each squared error is  $(u_{ik})^m$ , the mth 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)

 $\sum_{i=1}^{c} (u_{ik})^{m} d_{ik}^{2} = \text{sum of squared } A\text{-errors due to } y_{k}s$ partial replacement by all c of the
centers  $\{v_{i}\}$  (7c)

 $\sum_{k=1}^{N} \sum_{i=1}^{c} (u_{ik})^{m} d_{ik}^{2} = \text{overall weighted sum of generalized}$  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  $m \to 1$  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  $m \to \infty$ . 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,  $1.5 \le m \le 3.0$  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  $\mathbb{R}^n$ . Because every norm on  $\mathbb{R}^n$  is inner product induced via the formula

$$\langle x, y \rangle_{A} = x^{T} A_{\nu}, \tag{8}$$

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

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

$$C_y = \sum_{k=1}^{N} (y_k - c_y)(y_k - c_y)^t,$$
 (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

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

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

$$A = C_{\nu}^{-1} \sim \text{Mahalonobis Norm.}$$
 (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 hyperellipsodial, 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

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

$$\hat{u}_{ik} = \left(\sum_{j=1}^{c} \left(\frac{\hat{d}_{ik}}{\hat{d}_{jk}}\right)^{2/(m-1)}\right)^{-1}; \quad 1 \le k \le N; \ 1 \le i \le c$$
(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  $U^{(o)} \in M_{fc}$ . Then at step k, k,  $= 0, 1, \ldots$ , LMAX
- (A) Compute means  $\hat{v}^{(k)}$ , i = 1, 2, ..., 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  $\|\hat{U}^{(k+1)} \hat{U}^{(k)}\| < \in$ , 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  $\{\hat{U}^{(k)}, \hat{v}^{(k)}, \hat{v}^{(k)},$ 

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

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

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

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

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

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

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  $\hat{U} \not\subseteq M_c$  (when  $a = e = 2.71 \cdot \cdot \cdot \cdot$ ).

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):

ICON = 1 
$$\Rightarrow$$
 A = I  
ICON = 2  $\Rightarrow$  A =  $D_y^{-1}$ .  
ICON = 3  $\Rightarrow$  A =  $C_y^{-1}$ .

Other parameters read are:

QQ = Weighting exponent m: 1 < QQ.

KBEGIN = Initial number of clusters:

 $2 \le KBEGIN \le DCEASE$ .

KCEASE = Final number of clusters:

KCEASE < NS.

At any step 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  $\in$  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  $c_v$  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  $\hat{u}/s$  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 = 
$$\max_{i,k} \{ |\hat{u}_{ik}^{(k+1)} - \hat{u}_{ik}^{(k)}| \} < \text{EPS}.$$
 (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,  $(N \ge n)$ , 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  $n \le N$ . 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 Indicants. 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  $F_c$ ,  $1 - F_c$ ,  $H_c$ ,  $J_m$ ,  $\{\hat{v}_i\}$ , and  $\hat{U}$  are printed.

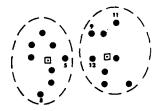
Output Summary. The final block of FCM outputs statistics for the entire run.

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  $\mathbb{R}^2$ . This artificial data set was originally published in Sneath



No.	Coordinates	
	y <sub>k1</sub>	y <sub>k2</sub>
1 2 3 4 5 6 7 8	0 0 1 2 3 2 2	4 3 5 4 3 2 1
9 10 11 12 13 14 15	5 6 7 5 7 6 6	5 6 3 3 2 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	<b>EPS</b> = ∈
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:

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

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

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

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

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

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	ICON = 1	ICON = 2	ICON = 3
Point	A = I	$A = D_y^{-1}$	A = C <sub>y</sub> -1
1	0.92	0.88	0.89
1 2 3 4 5 6 7 8	0.95	0.93	0.92
3	0.86 0.91	0.78 0.88	0.82 0.93
5	0.80	0.84	0.93
6	0.95	0.88	0.82
7	0.86	0.72	0.85
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 13	0.10 0.02	0.08 0.03	0.09 0.04
14	0.06	0.03	0.06
15	0.16	0.24	0.19
16	0.15	0.21	0.19
Ŷ <sub>11</sub>	6.18	5.99	5.96
Ŷ <sub>12</sub>	3.15	2.95	2.75
Ŷ <sub>21</sub>	i.44	1.67	1.73
Ŷ <sub>22</sub>	2.83	3.01	3.19
F <sub>c</sub>	0.80	0.71	0.71
н <sub>С</sub>	0.35	0.45	0.45
ງ <sub>m</sub>	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	
1 2 3 4 5 6 7 8	1.00	0.95 0.86	
4	1.00	0.91	
5	1.00	0.80	
6	1.00	0.95	
/	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 13	0.00	0.10 0.02	
14	0.00	0.06	
15	0.00	0.16	
16	0.00	0.15	
Ŷ <sub>11</sub>	6.25	6.18	
₹ <sub>12</sub>	3.25	3.15	
	1.37	1.44	
v <sub>21</sub> v <sub>22</sub>	2.75	2.83	
F <sub>c</sub>	1.00	0.80	
H_	0.00	0.35	
Jm	60.35	51.65	
Iter.	4	6	

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

Weighting	Number of	Partition	Lower	Normalized
Exponent	Clusters	Coefficient	Bound	Entropy
(m)	(c)	(F <sub>C</sub> )	(1-F <sub>c</sub> )	(H <sub>C</sub> )
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 Mahalonobis 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

```
00001000
C
                                                                          00002000
                                                                           000C3000
      THIS IS THE FCM (FUZZY C-MEANS) ROUTINE. THIS LISTING IS FOR A
CCC
      IBM TYPE COMPUTER WITH A FORTRAN IV COMPILER. IT ADAPTS FOR ANY
                                                                           00004000
      FORTRAN COMPILER WITH MODIFICATIONS SET AT THE USER SITE.
                                                                           00005000
                                                                           00000000
0000
      REFERENCE: "PATTERN RECOGNITION WITH FUZZY OBJECTIVE FUNCTIONS,"
                                                                           00007000
                                                                           0008000
                  JAMES BEZDEK, PLENUM, NEW YORK, 1981.
                                                                           00009000
С
                                                                           00010000
      DESCRIPTION OF OPERATING VARIABLES:
                                                                           00011000
CCC
      I. INPUT VARIABLES (FROM FILE 5)
                                                                           00012000
          CARD 1:
                                                                           00013000
           TITLE (20) ...... 80 CHARACTER HEADING
                                                                           00014000
00015000
          CARD 2:
           FMT(20).....FORTRAN FORMAT (CONTAINED IN PARENTHESIS)
                                                                           00016000
                             DESCRIBING THE INPUT FORMAT FOR THE RAW DATAGOOT7000
                             UP TE 80 CHARACTERS MAY BE USED
                                                                           00018000
                                                                           00019000
           COL 1: ICON.....DISTANCE MEASURE TO BE USED. IF: ,
                                                                           00020000
                             ICON=1 USE EUCLIDEAN NORM
                                                                           00021000
                             ICON=2 USE DIAGONAL NORM
                                                                           00022000
                                                                           00023000
                             ICON=3 USE MAHALANOBIS NORM
           COLS 2-7: QQ.....WEIGHTING EXPONENT FOR FCM
                                                                           00024000
           COLS 8-9: ND....NUMBER OF FEATURES PER INPUT VECTOR
                                                                           00025000
```

```
COLS 10-11: KBEGIN. STARTING NUMBER OF CLUSTERS
                                                                     00026000
Č
          COLS 12-13:KCEASE.FINISHING NUMBER OF CLUSTERS (NOTE: KBEGIN 00027000
                     MUST BE LESS THAN OR EQUAL TO KCEASE) 00028000
                                                                      00029000
С
          Y(NS,ND).....FEATURE VECTORS, INPUT ROW-WISE
                                                                      00030000
     II. INTERNAL VARIABLES
                                                                      00031000
          NS.....NUMBER OF DATA VECTORS
                                                                     00032000
          EPS..... MAXIMUM MEMBERRSHIP ERROR AT CONVERGENCE
C.
                                                                     00033000
          NC.....CURRENT NUMBER OF CLUSTERS
                                                                      00034000
          LMAX..... WAXIMUM NUMBER OF ITERATIONS WITHOUT
                                                                     00035000
                      CONVERGENCE
C
                                                                      00036000
         FM(ND).....SAMPLE MEAN VECTOR
                                                                      00037000
         FVAR(ND).....VECTOR OF MARGINAL VARIANCES
                                                                     00038000
         CC(ND, ND)......SCALING MATRIX
AA(ND, ND)......SAMPLE COVARIANCE MATRIX
С
                                                                     00039000
                                                                      00040000
         AI(ND, ND)......INVERSE OF SAMPLE COVARIANCE MATRIX
                                                                     00041000
         BB(ND).....DUMMY FGLDING MATRIX
CCC(ND).....DUMMY HGLDING MATRIX
                                                                      00042000
С
                                                                     00043000
         ST(ND, ND)......DUMMY FOLDING MATRIX FOR AA
                                                                      00044000
         CM(ND, ND).....CM=AA*(AA INVERSE)
U(NC, NS).....MEMBERSHIP MATRIX
                                                                      00045000
C.
                                                                      00046000
         W(NC,NS)....updated membership matrix
                                                                     00047000
          V(NC, ND)......CLUSTER CENTERS
                                                                      00048300
         ITT(NC).....DUMMY FOLDING MATRIX
                                                                      00049000
         H(NC).....ENTROPY MATRIX
¢
                                                                      00050000
          VJM(NC).....PAYOFF MATRIX
                                                                     00051000
          F(NC).....MATRIX OF PARTITION COEFFICIENTS
С
                                                                     00052000
          DIF(NC).....MATRIX OF ENTROPY BOUNDS
C
                                                                     00053000
С
                                                                      00054000
                                                                      00055000
```

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

```
DIMENSION FM(50), FVAR(50), F(20)
                                                        00057000
    DIMENSION BB(50),CCC(50),H(20),DIF(20),ITT(20)
                                                        00058000
    DIMENSIGN Y(500,2),U(20,500),W(20,500)
                                                        00059000
    DIMENSION AA(50,50),AI(50,50)
                                                        00060000
    DIMENSION CC(50,50), CM(50,50), ST(50,50)
                                                        00061000
    DIMENSION V(20,50), VJM(20)
                                                        00062000
    DIMENSION FMT(20), TITLE(20)
                                                        00063000
    READ(5,1458) (TITLE(I),I=1,20)
                                                        00064060
1458 FORMAT(20A4)
                                                        00065000
    READ(5,12321) (FMT(I), I=1,20)
                                                        00066000
12321 FORMAT(20A4)
                                                        00067000
    CONTROL PARAMETERS.
                                                        00069000
EP S= • 01
    NS = 1
                                                        00072000
    LMAX=50
                                                        00073000
                     READ FEATURE VECTORS (Y(1,J)).
                                                        00075000
C
     C----
    READ(5,2021) ICON,QQ,ND,KBEGIN,KCEASE
                                                        00077000
2021 FORMAT(11,F6.3,312)
                                                        00078000
    WRITE(6,410)
                                                        00079000
    FORMAT(///1H , *** *** BEGIN FUZZY C-MEANS OUTPUT *** ****)
WRITE(6,1459) (TITLE(III), III=1,20)
410
                                                        00080000
                                                        00081000
1459 FORMAT(10X,20A4///)
                                                        00082000
    READ(5,399,END=3)(Y(NS,J),J=1,ND)
                                                        00083000
    FORMAT (2F1.0)
399
                                                        00084000
    WRITE(6,12738)(Y(NS,J),J=1,ND)
                                                        00085000
12738 FORMAT(2(10X,10(F7.2,1X)/))
                                                        00086000
                                                        00087000
    NS = NS + 1
    GO TO 1
                                                        00088000
    NS=NS-1
                                                        00089000
    ND I M= ND
                                                        00090000
    NSAMP=NS
                                                        00091000
    WRITE(6,11111) NSAMP
                                                        00052000
11111 FORMAT(10X, 'NUMBER OF SAMPLES = ',15)
                                                        00093000
    ANSAMP=NSAMP
                                                        00054000
                     SCALED NORM REQUIRED IN STATEMENTS 31 AND 33.
                                                       000 960 00
С
    CALCULATION OF SCALING MATRIX FOLLOWS.
                                                        00097000
C.
    FEATURE MEANS.
                                                        00098000
C-----
```

```
00 350 I=1,NDIM
                                                           00100000
                                                           001 01000
    FM([]=0.
                                                           001 02 0 00
    DO 351 J=1.NSAMP
    FM(I) = FM(I) + Y(J \cdot I)
                                                           001 C3 0 0 0
351
                                                           00104000
350
    FM(I)=FM(I)/ANSAMP
C--
                         00106000
C.
     FEATURE VARIANCES.
                      C --
    DO 352 I=1.NDIM
                                                           001 C8000
    FVAR([)=0.
                                                           00109000
    00 353 J=1.NSAMP
                                                           00110000
FILE: KMEANS FCRTRAN A 03/18/83 11:05 VM/SP CONVERSATIONAL MCNITOR SYSTEM
```

```
353
      FVAR(I)=FVAR(I)+((Y(J,I)-FM(I))**2)
                                                                        00111000
352
      FVAR(I)=FVAR(I)/ANSAMP
                                                                        00112000
      IF(ICON-1)380,380,382
                                                                        00113000
      DO 381 I=1,NDIM
DO 381 J=1,NDIM
380
                                                                        00114000
                                                                        00115000
381
      CC(I,J)=0.
                                                                        00116000
      DO 370 I=1.NDIM
                                                                        00117000
      CC(I,I)=1.
370
                                                                        00118000
      GO TO 390
                                                                        00119000
382
      IF(ICON-2)384,384,386
                                                                        00120300
      DO 385 I=1,NDIM
384
                                                                        00121000
      DO 385 J=1.NDIM
                                                                        00122000
      CC(I,J)=0.
385
                                                                        00123000
      DO 371 I=1.NDIM
                                                                        00124000
      CC(I, I)=1./FM(I)
371
                                                                        001.25000
      GO TO 390
                                                                        00126000
      DO 360 I=1,NDIM
386
                                                                        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 [=1,NDIM
                                                                        001330C0
      DO 550 J=1,NDIM
                                                                        001 340 00
550
      ST(I,J)=AA(I,J)
                                                                        00135000
Ç-
                                           -----00136000
      INVERSION OF COVARIANCE MATRIX AA TO AI
C
                                                                        00137000
C----
        NN=NDIM-1
                                                                        001 39000
      AA(1,1)=1./AA(1,1)
                                                                        00140000
      DO 500 M=1.NN
                                                                        00141000
      K = M + 1
                                                                        00142000
      00 501 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
                                                                        00147000
      D=0.
      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
      AA(I,K) = -BB(I) * AA(K,K)
                                                                        00153000
503
                                                                        00154060
      DD 504 J=1,M
      CCC(J)=0.
                                                                        00155000
      DO 504 I=1.M
                                                                        00156000
504
                                                                        00157000
      CCC(J)=CCC(J)+AA(K,I)*AA(I,J)
      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
      AA(I,J) = AA(I,J) - BB(I) * AA(K,J)
500
                                                                        00162000
      DO 520 I=1,NDIM
                                                                        00163000
      DO 520 J=1,NDIM
                                                                        00164300
      AI(I,J)=AA(I,J)
520
                                                                        00165000
```

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

00239000 00240000

```
C--
С
DO 530 I=1,NDIM
                                                             00172000
     DO 530 J=1,NDIM
     CM(1,J)=0.
                                                             00174000
     DO 530 K=1.NDIM
                                                             00175000
    CM(I,J)=CM(I,J)+ST(I,K)*AI(K,J)
                                                             00176000
     WRITE(6,531)
                                                             J0177000
    FORMAT(' ',//,' CHECK MATRIX Al*AA=1, THE IDENTITY'//)
531
                                                             00178000
     DO 532 I=1,NDIM
                                                             00179000
     WRITE (6,533) (CM(I,J),J=1,NDIM)
532
                                                             00180000
     FORMAT(10X, 20F6.2)
533
                                                             00181000
     WRITE(6,1460) (TITLE(III), III=1,20)
                                                             00182000
390
1460 FORMAT('1',10X,20A4///)
                                                             00183000
     WRITE(6,420)
                                                             00184000
     FORMAT(' ',///,15X,'SCALING MATRIX CC',///)
420
                                                             00185000
     DO 421 I=1, NDIM
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(////)
                                                             001 90000
C----
      QQ IS THE BASIC EXPONENT FOR FUZZY ISODATA.
00194000
     PP=(1./(QQ-1.))
     DO 55555 NCLUS=KBEGIN, KCEASE
                                                             00155000
     WRITE(6,1460) (TITLE(III),III=1,20)
                                                             00196000
     WRITE(6,499) NCLUS, ICON, QQ
                                                             001 57000
     FORMAT(' ',' NUMBER OF CLUSTERS = ',13,5X,' ICON = ',13,5X, 00198000
    C'EXPONENT = ',F4.2,//)
                                                             001 99000
                                                             00200000
                                                          ----00201000
   RANDOM INITIAL GUESS FOR U(I,J)
    THE RANDOM GENERATOR SUBROUTINE RANDU FROM THE IBM SCIENTIFIC 00203000 SUBROUTINE PARKACE (SERVICE AND TO THE IBM SCIENTIFIC 00203000
С
С
    SUBROUTINE PACKAGE (SSP) IS USED AND IS CALLED FROM AN EXTERNAL
LIBRARY. DTHER GENERATORS THAT PRODUCE VALUES ON THE INTERVAL
22FO TO ONE CAN BE USED.
С
С
    ZERO TO ONE CAN BE USED.
      RANDOM=.7731
                                                              002 080 00
     I X = 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(1,K)=S*(1.0-RANDOM**(1.0/ANC))
                                                             00218000
1101 S= S-U(I,K)
1100 U(NCLUS,K)=S
                                                              30219000
                                                              00220000
FILE: KMEANS FORTRAN A 03/18/83 11:05 VM/SP CONVERSATIONAL MONITOR SYSTEM
                         ______00221000
C CALCULATION OF CLUSTER CENTERS V(1).
C------
                                                              00224000
7000 DO 20 I=1.NCLUS
                                                              00225000
     DO 20 J=1,NDIM
                                                              00226000
     V( I, J)=0.
                                                              00227000
     00 21 L=1,NSAMP
                                                              00228000
     V(I,J)=V(I,J)+((U(I,L)**Q)*Y(L,J))
                                                              00229000
                                                              00230000
     D=D+(U(I,L)**QQ)
    V(I,J)=V(I,J)/D
                                                              00231000
20
                              _____00232000
C.--
                                                              00233000
    UPCATE MEMBERSHIP FUNCTIONS.
                             ______002 340 00
                                                              00235000
6111 DO 38 I=1, NCLUS
     DO 38 J=1, NSAMP
                                                              00237000
     0 = (L, I)W
                                                              00238000
     A=0.
     DO 31 L=1,NDIM
```

DO 31 M=1,NDIM

```
JAMES C. BEZDEK, ROBERT EHRLICH, and WILLIAM FULL
31
     A=A+((Y(J,L)-V(I,L))*CC(L,M)*(Y(J,M)-V(I,M)))
                                                                   00241000
     A=1./(A**PP)
                                                                   00242000
                                                                   00243000
      SUM=0.
     DO 32 N=1, NCLUS
                                                                   00244000
     C=0.
                                                                   00245000
     DO 33 L=1.NDIM
                                                                   00246000
     00 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
     MU2\A=(L,I)W
                                                                   00251000
     CONTINUE
38
                                                                   00252000
                                                           ------00253000
     FRROR CRITERIA AND CUTOFFS.
                                                                  00254000
C.
C----
     9000 ERRMAX=0.
                                                                   00256000
     00 40 [=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
    FORMAT(1H , 'ITERATION = ',14,5x,'MAXIMUM ERROR = ',F10.4,
110x,'NUMBER OF CLUSTERS = ',14)
400
                                                                   00263000
                                                                   00264000
     DO 42 I=1,NCLUS
                                                                   00265000
     DO 42 J=1, NSAMP
                                                                   00266000
     U(I,J)=W(I,J)
42
                                                                   00267000
     IF(ERRMAX.LE.EPS) GO TO 6000
                                                                   00268000
43
     TT = TT + 1
                                                                   00269000
     IF(IT-LMAX) 7000,7000,6000
                                                                   00270000
                                                               ----00271000
С
     CALCULATION OF CLUSTER VALIDITY STATISTICS F, H, 1-E
                                                                  00272000
       C----
6000 ITT(NCLUS)=IT
                                                                   00274000
     F(NCLUS)=0.0
                                                                   00275000
FILE: KMEANS FORTRAN A 03/18/82 11:05 VM/SP CONVERSATIONAL MONITOR SYSTEM
                                                                    00276000
      H(NCLUS)=0.0
      DO 100 I=1, NCLUS
      DO 100 K=1,NSAMP
```

```
00277000
                                                                   00278000
                                                                   00279000
     AU=U(I,K)
                                                                   00280000
     F(NCLUS)=F(NCLUS)+AU**2/ANSAMP
                                                                   00281000
     IF (AU) 10C, 100, 101
                                                                   00282000
     H(NCLUS)=H(NCLUS)-AU*ALOG(AU)/ANSAMP
101
                                                                   00283000
100
     CONTINUE
                                                                   00284000
     DIF(NCLUS)=1.0-F(NCLUS)
                                 c.
     CALCULATION OF OBJECTIVE FUNCTION
                                                                   00286000
C
                                                                ----00287000
C----
           00288000
     \Delta = 0
                                                                   00289000
     DO 80 [=1,NCLUS
                                                                   002 90000
     00 80 J=1,NSAMP
                                                                   00251000
     DIST=0.
                                                                   00292000
     DO 81 L=1,NDIM
                                                                   002 $3000
     DO 81 M=1,NDIM
     DIST=DIST+((Y(J,L)-V(I,L)) +CC(L,M)+(Y(J,M)-V(I,M)))
                                                                   002 940 00
81
                                                                   00295000
     A=A+(\{U\{I,J\}++QQ\}+DIST)
                                                                   00296000
80
     VJM(NCLUS)=A
                                                         ----------002 97000
c-
                                                                   00298000
     OUTPUT BLOCK FOR CURRENT NCLUS
C
                   ______00259000
                                                                   00300000
     WRITE(6,401)
     FORMAT(! '///' FSTOP',7X,'1-FSTOP',5X,'ENTROPY',5X,'PAYOFF',5X,/) 00301000
401
                                                                   00362000
     WRITE(6,699) F(NCLUS), DIF(NCLUS), H(NCLUS), VJM(NCLUS)
                                                                   00303000
     FORMAT(1H ,2(F6.3,4X),4X,F6.3,5X,E8.3)
699
                                                                   003 040 00
     WRITE(6,59)
                                                                   00305000
59
     FORMAT(1X,100('-')//)
     WRITE(6,402)
                                                                   00366000
                                                                   00307000
402
     FORMAT(///,15x, 'CLUSTER CENTERS V(I,J)',///>
                                                                   003 C8 0 0 0
     DO 415 I=1, NCLUS
                                                                   00309000
415
     WRITE(6,404) (I,J,V(I,J),J=1,ND[M)
404
     FORMAT(' 1=',[3,3X,'J=',[3,3X,'V([,J)=',F8.4)
                                                                   00310000
     FORMAT(1H ,7(F6.4,3X))
                                                                   00311000
405
                                                                   00312000
     WRITE(6,59)
                                                                   00313000
     WRITE(6,406)
```

00351000

```
00314000
406
      FORMAT(1H ,///,25X, 'MEMBERSHIP FUNCTIONS',///)
                                                                      00315000
     00 407 J=1,NSAMP
                                                                      00316000
407
     WRITE(6,408) J, (U(I,J), I=1, NCLUS)
                                                                      00317000
     FORMAT(1H ,'J=',13,5X,8(F6.4,3X))
408
54444 CONTINUE
                                                                      00318000
                                                                      00319000
55555 CONTINUE
             00321000
     OUTPUT SUMMARY FOR ALL VALUES OF C
C
          _______0322000
C-
                                                                      00323000
                                                                      00324000
450
     FORMAT('1',25X, 'RUN SUMMARY')
                                                                      00325000
     WRITE(6,460) NSAMP
     FORMAT( ' '//' NUMBER OF SUBJECTS N = ', 14)
                                                                      00326000
460
                                                                     00327000
     WRITE(6,461) NDIM
     FORMAT(1HO, NUMBER OF FEATURES NDIM = 1,14)
                                                                     003 28 0 0 0
461
                                                                     00329000
     WRITE(6,462) EPS
     FORMAT(1HO, MEMBERSHIP DEFECT BOUND EPS = 1,F6.4)
                                                                     00330000
462
FILE: KMEANS FORTRAN A 03/18/83 11:05 VM/SP CONVERSATIONAL MONITOR SYSTEM
                                                                      00331000
      WRITE(6,464) ICON
      FORMAT(1HO, NORM THIS RUN ICCN = ', I1)
                                                                      00332000
 464
                                                                      00333000
      WRITE(6,465) QQ
      FORMAT(1HO, WEIGHTING EXPONENT M = . 1, F4.2)
                                                                      00334000
 465
                                                                      00335000
      IF(IT.LE.49) GO TO 476
      WRITE(6,70107)
                                                                      00336000
 70107 FORMAT( * . CONVERGENCE FLAG: UNABLE TO ACHIEVE SATISFACTORY CLUST00337000
                                                                      00338000
      1ERS AFTER 50 ITERATIONS.')
                                                                      00339000
      WRITE(6,466)
 476
      FORMAT(' '//' NO. OF CLUSTERS',3X,'PART. COEFF.',5X, C'LOWER BOUND',5X,'ENTROPY',5X,'NUMBER OF ITERATIONS')
                                                                      00340000
 466
                                                                     00341000
                                                                     00342000
      WRITE(6.467)
                                                                      00343000
      FORMAT(1H0,6X,'C',17X,'F',15X,'1-F',12X,'H',10X,'IT')
 467
                                                                     00344000
      DO 468 J=KBEGIN, KCEASE
      WRITE(6,469) J,F(J),DIF(J),F(J),ITT(J)
                                                                      00345000
 468
      FORMAT(1H ,6X,12,14X,F6.3,11X,F6.3,7X,F6.3,8X,14)
                                                                      00346000
 469
                                                                      00347000
 55556 CONTINUE
                                                                      00348000
       WRITE(6,411)
 616
       FORMAT(////1H , **** *** NORMAL END OF JOB *** ****)
                                                                      00349000
 411
                                                                      00350000
```

STOP

END