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Convex Decompositions of Fuzzy Partitions*

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In this paper we investigate some algebraic and geometric properties of fuzzy partition spaces (convex hulls of hard or conventional partition spaces). In particular, we obtain their dimensions, and describe a number of algorithms for effecting convex decompositions. Two of these are easily programmable, and each affords a different insight about data structures suggested by the fuzzy partition decomposed. We also show how the sequence of partitions in any convex decomposition leads to a matrix for which the norm of the corresponding coefficient vector equals a scalar measure of partition fuzziness used with certain fuzzy clustering algorithms.

I. INTRODUCTION AND CONCLUSIONS

The clustering algorithms of Ruspini [1], Woodbury [2], Bezdek [3], and Dunn [4] all yield fuzzy partitions as clustering solutions for partitioning finite data sets. It was shown in [3] that fuzzy partition spaces are minimal convex supersets, that is, convex hulls, of hard (or conventional) partition spaces. Our goal in this paper is to explore some of the algebraic and geometric consequences of this convexity property.

Partition spaces are defined in Section II; some previous results and several new observations are given. Section III contains our proof that the space of fuzzy c-partitions on n data points has dimension $n(c - 1)$. In IV an algorithm using a minimax strategy is defined and illustrated numerically. We show that minimax decompositions have lexicographically optimal coefficients. A second decomposition is given in V that interprets the construction of fuzzy partitions from a

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sequence of hard ones as a sequence of transitions or reclassifications from a state of "maximum membership." In VI the partition coefficient used in [5] for evaluation of cluster validity is related to convex decompositions: we prove that this measure of fuzziness is proportional to the number of reclassifications made in the terms of every decomposition of the fuzzy partition in question. This result lends additional support to the clustering strategy proposed in [3] and [5].

II. Partition Spaces

Let $X = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\} \subset \mathbb{R}^s$ be a given finite data set. We fix the integer c, $2 \leqslant c < n$, and denote by V_{cn} the usual vector space of real $(c \times n)$ matrices. Suppose $P = (Y_1, Y_2, \ldots, Y_c)$ to be a conventional hard c-partition of X. Thus for each i, $1 \leqslant i \leqslant c$ we have $Y_i \subset X$; for each $i \neq j$ the intersection $Y_i \cap Y_j$ is empty; and the union of the Y_i's is all of X, $\bigcup_{i=1}^{c} Y_i = X$. We say that P is *non-degenerate* in case none of the Y_i's is empty, and is *degenerate* otherwise. Partitions of X can be conveniently characterized by matrices in V_{cn} as follows: let u_{ik} be the ik-th element of $U \in V_{cn}$, and define

$$P_c = \left\{ U \in V_{cn}\colon u_{ik} \in \{0, 1\}\ \forall\, i, k;\ \sum_{i=1}^{c} u_{ik} = 1\ \forall\, k;\ \sum_{k=1}^{n} u_{ik} > 0\ \forall\, i \right\}. \tag{1}$$

For U in P_c we interpret u_{ik} as the value of a characteristic function $u_i\colon X \to \{0, 1\}$; u_{ik} specifies the membership of $\mathbf{x}_k$ in a partitioning subset Y_i of X:

$$\begin{aligned} u_{ik} \doteq u_i(\mathbf{x}_k) &= 1; \qquad \mathbf{x}_k \in Y_i \\ &= 0; \qquad \text{otherwise.} \end{aligned} \tag{2}$$

The c-tuple $(u_1, u_2, \ldots, u_c)$ is the function-theoretic equivalent of $(Y_1, Y_2, \ldots, Y_c)$, so each $U \in P_c$ is uniquely identifiable with a hard c-partition of X via (2). Accordingly, we may call P_c ***hard c-partition space*** associated with X, and because degeneracy is manifested by zero rows in U, the superset

$$P_{c0} = \left\{ U \in V_{cn}\colon u_{ik} \in \{0, 1\}\ \forall\, i, k;\ \sum_{i=1}^{c} u_{ik} = 1\ \forall\, k;\ \sum_{k=1}^{n} u_{ik} \geqslant 0\ \forall\, i \right\} \tag{3}$$

is ***degenerate hard c-partition space*** for X.

P_c and P_{c0} are not "spaces" in any ordinary sense; rather, they are extremely large finite sets in the positive or non-negative orthant of V_{cn}. Since $|P_{c0}| < \infty$, exhaustive search for "optimal" partitions of X is theoretically possible, but infeasible in practice because of their cardinalities: e.g., $|P_c| \approx 10^{18}$ if $c = 10$, $n = 25$. Thus finiteness is an impediment to tractable algorithms as well as analytic techniques when partitioning of X is desired.

An even stronger objection to P_c lies with the physical interpretation of data substructure it requires. Every $\mathbf{x}_k$ in X belongs entirely to one and only one of the hard partitioning subsets u_i (since u_i and Y_i are equivalent, we may call u_i a set). All members of u_i are fully related to each other, and at the same time totally unrelated to all other members of the data because the boundaries of the partitioning subsets are hard. This is a particulary harsh model for many physical processes, since data representative of most situations originates from mixed populations. It seems more realistic to allow individuals to *share memberships* in several partitioning subclasses (for example, this is the situation we anticipate for data representing hybrids in mixtures of biological species at the same strata).

A natural way to ameliorate these objections was suggested by Zadeh in [6], who proposed that non-statistical uncertainties of the type described above might be more accurately represented by allowing memberships in *fuzzy sets*, characterized by membership *functions* valued in [0, 1]. Motivated by these considerations, and using (1) as our guide, we define

$$P_{fc} = \left\{ U \in V_{cn}: u_{ik} \in [0, 1] \; \forall\, i, k; \sum_{i=1}^{c} u_{ik} = 1 \; \forall\, k; \sum_{k=1}^{n} u_{ik} > 0 \; \forall\, i \right\} \tag{4}$$

as *fuzzy, non-degenerate c-partition space* for X. Here u_{ik} is again the *grade of membership* of $\mathbf{x}_k$ in the fuzzy subset u_i: $X \to [0, 1]$. The condition $\sum_{i=1}^{c} u_{ik} = 1$ for each k insures that each $\mathbf{x}_k$ has unit membership (in X); these memberships may be distributed among the c fuzzy subsets $\{u_i\}$ arbitrarily as long as their sum is unity. Corresponding to P_{c0} in the hard case is *degenerate fuzzy c-partition space* P_{fc0} obtained from (4) by relaxing the last condition exactly as was done in (3); P_{fc0} is not used in the sequel.

A substantial amount of information concerning the imbeddings $P_c \subset P_{c0} \subset P_{fc} \subset P_{fc0}$ is available elsewhere [3]. The main fact established there we intend to exploit below is that P_{fc} is the convex hull of P_{c0}, $P_{fc} = \operatorname{conv}(P_{c0})$. We observe that the convex hull of P_c is a proper subset of $\operatorname{conv}(P_{c0})$, by noting that, for example, with any λ in [0, 1] the matrix

$$U = \begin{bmatrix} \lambda & \lambda & \lambda \\ 1 - \lambda & 1 - \lambda & 1 - \lambda \end{bmatrix} \tag{5}$$

lies in $\operatorname{conv}(P_{20})$, but is not in $\operatorname{conv}(P_2)$. In other words, this U has no convex decomposition with all non-degenerate terms. The additional property U in P_{fc} needs to distinguish it as a member of $\operatorname{conv}(P_c)$ is not yet known: our interest lies with P_{fc} due to the physical considerations outlined above.

III. The Dimension of Fuzzy Partition Space

In this section we prove that the dimension of P_{fc} is $n(c-1)$, $\dim(P_{fc}) = n(c-1)$. P_{fc} is convex, so takes its dimension from the vector subspace which translates the affine hull of P_{fc} to the origin of V_{cn}; $\dim(P_{fc}) = \dim(M)$, where $\mathit{aff}(P_{fc}) = U^* + M$, $U^* \in V_{cn}$, and M a vector subspace in V_{cn}. Before stating and proving this theorem, we sketch the idea of the proof. Given $U \in P_{fc}$, one can choose any positive path $\mathbf{v}_j = (*_1, *_2, ..., *_n)$ with $*_i > 0$ for every i through the columns of U. Such a path is illustrated pictorially in (6):

$$U = \begin{bmatrix} u_{11} & u_{12} & \cdots\cdots & \boxed{u_{1k} = *_k} & \cdots\cdots & u_{1n} \\ u_{i1} & \boxed{u_{i2} = *_2} & \cdots\cdots & \cdots\cdots & \cdots\cdots & u_{in} \\ \boxed{u_{j1} = *_1} & \cdots\cdots & \cdots\cdots & \cdots\cdots & \cdots\cdots & u_{jn} \\ u_{c1} & u_{c2} & \cdots\cdots & \cdots\cdots & \cdots\cdots & \boxed{u_{cn} = *_n} \end{bmatrix}. \tag{6}$$

Call c_j the smallest element of $\mathbf{v}_j$; define a matrix $U_j \in P_{c0}$ to have 1's at every address of the entries of $\mathbf{v}_j$, and 0's elsewhere. Define a residual matrix $R_j = U - c_j U_j$. Apply this iteratively to R_j, beginning at $R_0 \doteq U$; we shall first show that $R_j \to \theta$ in $n(c-1)+1$ or less steps; and to complete the proof, that there is a matrix in P_{fc} which cannot be decomposed with less than $n(c-1)+1$ terms. This will prove

THEOREM 1. *For P_{fc} as defined in* (5), *we have*

$$\dim(P_{fc}) = n(c-1). \tag{7}$$

Proof. Let $U \in P_{fc}$. For $1 \leqslant k \leqslant n$ choose i_k so that the entries $u_{i_k,k} > 0$, and set $U = R_0$, $I_1 = \{i_k : 1 \leqslant k \leqslant n\}$. This is always possible because columns of U must sum to 1, so every column has at least one non-zero entry. Define the n-vector $\mathbf{v}_1 = (u_{i_1,1}, u_{i_2,2}, ..., u_{i_n,n})$, and set $c_1 = \min_{I_1}\{u_{i_k,k}\}$. If $c_1 = 1$, U is already hard and we are done. Otherwise, define the matrix $U_1 \in P_{c0}$ via

$$\begin{aligned} (u_1)_{i_k,k} &= 1; \qquad i_k \in I_1 \\ &= 0; \qquad \text{otherwise,} \end{aligned} \tag{8}$$

so that U_1 has 1's wherever $\mathbf{v}_1$ passes through U, and 0's elsewhere. Next, define the residual matrix

$$R_1 = U - c_1 U_1 = R_0 - c_1 U_1. \tag{9}$$

Note that every column of R_1 sums to $1 - c_1 > 0$; moreover, R_1 contains at least one zero, viz., at the address where c_1 occured in U (it may have more than one zero if $\min_{I_1}\{u_{i_k,k}\}$ is not unique).

Proceeding iteratively, we apply the steps above to R_1: find a non-zero path $\mathbf{v}_2$ through its columns, factor out the smallest element $-c_2$ — in the path; define $U_2 \in P_{c0}$ using these path addresses, and set $R_2 = R_1 - c_2U_2$. Either R_2 is the zero matrix and we are done, or (i) column sums of R_2 are equal to $1 - (c_1 + c_2) > 0$, and (ii) R_2 has at least two zeores.

Continuing inductively, we have at the j-th step the residual $R_j = U - \sum_{k=1}^{j} c_kU_k$, and if R_j is not the zero matrix, then (i) column sums of R_j are positive, $\sum_{i=1}^{c} (r_j)_{ik} = 1 - \sum_{k=1}^{j} c_k$, and (ii) R_j has at least j zeroes. Now let $m = n(c - 1)$. Either this process terminates at some $j \leqslant m$, or after m iterations the residual R_m has at least m zeroes. If R_m is not the zero matrix, its positive column sums are $1 - \sum_{k=1}^{m} c_k > 0$, so every column has a non-zero entry. But $m = n(c - 1)$, so each column of R_m has exactly *one* entry which must equal $1 - \sum_{k=1}^{m} c_k$. Define $c_{m+1} = 1 - \sum_{k=1}^{m} c_k$, and $U_{m+1} \in P_{c0}$ using the addresses of the entries in R_m in the usual way. Then $R_{m+1} = U - \sum_{k=1}^{m+1} c_kU_k =$ the zero matrix. Since $\sum_{k=1}^{m+1} c_k = 1$ with all of the c_k's in (0, 1) and all of the U_k's $\in P_{c0}$, the convex decomposition of U is complete.

We have shown that every $U \in P_{fc}$ admits at least one convex decomposition with $n(c - 1) + 1$ terms. Thus by Caratheodory's theorem for convex sets (cf. Roberts and Varberg [7]), we conclude that $\dim(P_{fc}) \leqslant n(c - 1)$.

To complete the proof we must show that equality prevails. Towards this end, let $k \in \mathbb{R}$ and define $U = [u_{ij}]$ by

$$u_{ij} = \frac{k}{(2m)^{n(i-1)+(j-1)}}; \qquad 1 \leqslant i \leqslant c-1 \quad \text{and} \quad 1 \leqslant j \leqslant n$$
$$= 1 - \sum_{s=1}^{c-1} u_{sj}; \qquad i = c \quad \text{and} \quad 1 \leqslant j \leqslant n, \tag{10}$$

where again $m = n(c - 1)$. For $k \in (0, 1)$ this matrix belongs to P_{fc}. Suppose this U can be decomposed in less than or equal to m terms, say for convenience that $U = \sum_{j=1}^{n} \sum_{i=1}^{c-1} c_{ij}U_{ij}$, where $U_{ij} \in P_{c0}$, $c_{ij} \in [0, 1]$ $\forall\, i, j$, and $\sum_{j=1}^{n} \sum_{i=1}^{c-1} c_{ij} = 1$. To write $u_{11} = k$ as a partial sum of the convex coefficients, it is necessary that at least one of the c_{ij}'s is contained in the closed interval $[(1/m)\, k, k]$. We can assume without loss that c_{11} is this coefficient. Similarly, there is for u_{12} at least one of the c_{ij}'s, say c_{12}, so that $c_{12} \in [(1/m)\,(k/2m), (k/2m)]$, and $c_{11} \neq c_{12}$, because

$$\left[\left(\frac{1}{m}\right)(k), k\right] \cap \left[\left(\frac{1}{m}\right)\left(\frac{k}{2m}\right), \left(\frac{k}{2m}\right)\right] = \varnothing \qquad \text{for } k > 0.$$

Continuing inductively, it is clear that each u_{ij} in (10) for $1 \leqslant i \leqslant c-1$ and $1 \leqslant j \leqslant n$ requires a distinct coefficient c_{ij} which satisfies

$$c_{ij} \in \left[\left(\frac{1}{m}\right)\left(\frac{k}{(2m)^{n(i-1)+(j-1)}}\right), \left(\frac{k}{(2m)^{n(i-1)+(j-1)}}\right)\right]; \tag{11a}$$

$$c_{ij} \neq c_{st} \qquad \text{unless} \qquad i = s \quad \text{and} \quad j = t. \tag{11b}$$

In view of (11a), we can bound above the sum of these m c_{ij}'s by summing the upper endpoints of the intervals at (11a):

$$\sum_{j=1}^{n}\sum_{i=1}^{c-1} c_{ij} \leqslant \sum_{j=1}^{n}\sum_{i=1}^{c-1}\left\{\frac{k}{(2m)^{n(i-1)+(j-1)}}\right\}$$

$$= k\left\{1 + \frac{1}{(2m)} + \frac{1}{(2m)^2} + \cdots + \frac{1}{(2m)^{m-1}}\right\}$$

$$= k\left\{\frac{1-\left(\frac{1}{2m}\right)^m}{1-\left(\frac{1}{2m}\right)}\right\}.$$

If we choose k so that

$$k < \left\{\frac{1-\left(\frac{1}{2m}\right)}{1-\left(\frac{1}{2m}\right)^m}\right\}; \qquad m = n(c-1), \tag{12}$$

then $\sum_{j=1}^{n}\sum_{i=1}^{c-1} c_{ij} < 1$, and we need at least one more coefficient to effect a convex decomposition of U. That is, we *must* use $m + 1$ terms for the matrix at (10). Given c and n, it is clear from (12) that k can always be chosen so that U in (10) belongs to P_{fc}, so the proof is complete. Q.E.D.

IV. Minimax Decomposition

Because the residual at each step in the algorithm used for the proof of Theorem 1 has at least one entry forced to zero, we call it a *forcing (or F) algorithm.* Not all convex decompositions are achieved with forcing algorithms, and we shall see in the next section that every $U \in P_{fc}$ can be decomposed without using an F algorithm. Many different F-decompositions of a given U will generally be possible, since the only constraint on the path $\mathbf{v}_j$ in the above proof was positivity. Despite this problem of non-uniqueness, there is among the F-decompositions of U one which deserves special attention. If at each step the path $\mathbf{v}_j$ chosen through R_j is one of ***maximum*** residual memberships, the c_j factored from $\mathbf{v}_j$ will be the ***minimum maximum residual membership***, giving rise to the *Minimax* (*or MM*) *Decomposition.*

Let $U \in P_{fc}$. Following the algorithm given in the proof of Theorem 1, we modify the choice of path $\mathbf{v}_j$ as follows: at step $j+1$, choose $\mathbf{v}_{j+1}$ through R_j by letting (i_k, k) be the index at which $\max_{1 \leqslant i \leqslant 0}\{(r_j)_{ik}\}$ is achieved for $1 \leqslant k \leqslant n$. If more than one index occurs at any k, choose any one of these. Set $\mathbf{v}_{j+1} = (*_{i_1,1}, *_{i_2,2}, \ldots, *_{i_n,n})$, and $c_{j+1} = \min_{1 \leqslant k \leqslant n}\{(r_j)_{i_k,k}\}$. Then define $U_{j+1} \in P_{c0}$ to have 1's at the addresses from which the entries of $\mathbf{v}_{j+1}$ were chosen, and 0's elsewhere. Finally, put $R_{j+1} = R_j - c_{j+1}U_{j+1}$, and iterate until $R_k \to \theta$, the zero matrix.

To illustrate F-decompositions, we apply first an arbitrary F-algorithm, and then the MM-algorithm to the matrix

$$U = \begin{bmatrix} .90 & .80 & .30 & .40 & .05 \\ .10 & .20 & .70 & .60 & .95 \end{bmatrix}. \tag{13}$$

(i) *Arbitrary F-decomposition*

Since u_{ik} is positive for every i and k, we can extract at once any $c_1 = u_{ik}$. Arbitrarily choosing path $\mathbf{v}_1 = (*_{21}, *_{22}, *_{23}, *_{24}, *_{15})$ and taking for c_1 entry $u_{15} = .05$ leads to

$$c_1U_1 = .05\begin{bmatrix} 0 & 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{bmatrix};$$

and

$$R_1 = U - c_1U_1 = \begin{bmatrix} .90 & .80 & .30 & .40 & 0 \\ .05 & .15 & .65 & .55 & .95 \end{bmatrix}.$$

Choosing $c_2 = (r_1)_{21} = .05$ with $\mathbf{v}_2 = (*_{21}, *_{22}, *_{23}, *_{24}, *_{25})$ now yields

$$c_2U_2 = .05\begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix};$$

and

$$R_2 = \begin{bmatrix} .90 & .80 & .30 & 40 & 0 \\ 0 & .10 & .60 & .50 & .90 \end{bmatrix}.$$

Continuing in this fashion, one may generate various F-decompositions of U. For example, the paths and coefficients

$$\begin{aligned} c_3 &= .10{:} \quad \mathbf{v}_3 = (*_{11}, *_{22}, *_{23}, *_{24}, *_{25}) \\ c_4 &= .30{:} \quad \mathbf{v}_4 = (*_{11}, *_{12}, *_{13}, *_{14}, *_{25}) \\ c_5 &= .10{:} \quad \mathbf{v}_5 = (*_{11}, *_{12}, *_{23}, *_{14}, *_{25}) \\ c_6 &= .40{:} \quad \mathbf{v}_6 = (*_{11}, *_{12}, *_{23}, *_{24}, *_{25}) \end{aligned}$$

result in the particular decomposition

$$\begin{bmatrix} .90 & .80 & .30 & .40 & .05 \\ .10 & .20 & .70 & .60 & .95 \end{bmatrix}$$

$$= 0.5\begin{bmatrix} 0 & 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{bmatrix} \quad .05\begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix} + .10\begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 1 \end{bmatrix}$$

$$+ .30\begin{bmatrix} 1 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} + .10\begin{bmatrix} 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \end{bmatrix} + .40\begin{bmatrix} 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 \end{bmatrix}. \tag{14}$$

In (14) only U_2 is degenerate: the proportion of degenerate terms appearing in F-decompositions tends to increase with c. Moreover, there is little practical value for a decomposition like (14), since it furnishes no explanation or interpretation for structure in the fuzzy partition it decomposes.

(ii) *MM-decomposition*

Beginning again with U in (13), we find the initial minimax path $\mathbf{v}_1 = (*_{11}, *_{12}, *_{23}, *_{24}, *_{25})$ through U: the address yielding the MM membership is (2, 4), so $c_1 = u_{24} = .60$, thus

$$c_1U_1 = .60\begin{bmatrix} 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 \end{bmatrix};$$

and

$$R_1 = R_0 - c_1U_1 = U - c_1U_1 = \begin{bmatrix} .30 & .20 & .30 & .40 & .05 \\ .10 & .20 & .10 & 0 & .35 \end{bmatrix}.$$

Inspection of R_1 reveals that the residual MM membership is .20, that is, c_2 will be .20. There are, however, *two* MM paths which are available for this choice;

$$\mathbf{v}_2 = (*_{11}, *_{12}, *_{13}, *_{14}, *_{25}),$$

and

$$\mathbf{v}_2' = (*_{11}, *_{22}, *_{13}, *_{14}, *_{25}).$$

The choice of path is arbitrary, leading to either one of

$$c_2U_2 = .20\begin{bmatrix} 1 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \quad \text{or} \quad c_2U_2' = .20\begin{bmatrix} 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 \end{bmatrix}.$$

These choices would yield for residuals the matrices

$$R_2 = \begin{bmatrix} .10 & 0 & .10 & .20 & .05 \\ .10 & .20 & .10 & 0 & .15 \end{bmatrix} \quad \text{or} \quad R_2' = \begin{bmatrix} .10 & .20 & .10 & .20 & .05 \\ .10 & 0 & .10 & 0 & 15 \end{bmatrix}.$$

In either case, note that c_3 will be .10 and at step 3 there will be *four MM* paths available, two for each choice for R_2. All of these choices will leave residuals with minimax membership in R_3 equal to $c_4 = .05$. Finally, every branch at the fifth step would require the choice $c_5 = .05$. We exhibit one *MM* decomposition of U:

$$\begin{bmatrix} .90 & .80 & .30 & .40 & .05 \\ .10 & .20 & .70 & .60 & .95 \end{bmatrix}$$

$$= .60\begin{bmatrix} 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 \end{bmatrix} + .20\begin{bmatrix} 1 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} + .10\begin{bmatrix} 0 & 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 1 \end{bmatrix}$$

$$+ .05\begin{bmatrix} 1 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 0 & 0 \end{bmatrix} + .05\begin{bmatrix} 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 \end{bmatrix}. \tag{15}$$

Although the *MM*-decomposition (15) is non-unique, there are several important aspects of it that are invariant. In what follows it is convenient to introduce the following terminology:

DEFINITION 1. Let $\sum_{k=1}^{p} c_k U_k$ be any convex decomposition of U in P_{fc}. We call p the *length* of the decomposition, and the hard partition $U_j \in P_{c0}$ with $c_j = \max_{1 \leqslant k \leqslant p}\{c_k\}$ is called its *dominant term*. Since the sequence $\{c_k\}$ of coefficients generated by *MM*-algorithms is monotone decreasing by their definition, i.e., $1 \geqslant c_1 \geqslant c_2 \cdots \geqslant c_p > 0$, U_1 is *always* the dominant term in *MM* decomposition. In particular, this U_1 is the hard partition of X "closest" to U in the sense of maximum membership (cf. [5]), and deserves to be isolated by a special notation, say U_{mm}, because it is one whose structure can be readily interpreted as the best (in the sense of maximum membership) hard approximation to $U \in P_{fc}$.

Theorem 1 shows that the *MM*-algorithm terminates in at most $n(c - 1) + 1$ steps. In general, however, it may stop sooner, as was the case in our example above. Roughly speaking, this happens because we extract at each step the largest possible coefficient, thus yielding decompositions of minimal length. While *MM* decompositions are often non-unique, we may prove that both their lengths and coefficient sequences are:

THEOREM 2. *If $U \in P_{fc}$ has two distinct MM-decompositions, say $U = \sum_{k=1}^{p} c_k U_k = \sum_{k=1}^{q} c_k' U_k'$, then*

$$p = q; \tag{16a}$$

and

$$c_k = c_k' \qquad \forall\, 1 \leqslant k \leqslant p. \tag{16b}$$

Proof. Let M and N belong to V_{cn}, and set $I_c = \{1, 2,..., c\}$. We shall say that $M \cdot cp \cdot N$ iff for $1 \leqslant j \leqslant n$ there is a permutation $\pi_j: I_c \to I_c$ so that $m_{ij} = n_{\pi_j(i),j}$, $1 \leqslant i \leqslant c$. In other words, M and N can be obtained from each other by independently permuting the entries in corresponding columns.

Now let $U \in P_{fc}$ and suppose at the k-th step in MM-decomposition of U two distinct MM paths $\mathbf{v}_k$ and $\mathbf{v}_k'$ through R_{k-1} are available, yielding hard partitions $U_k \neq U_k'$. The values of $\mathbf{v}_k$ and $\mathbf{v}_k'$ are equal: it is their address origins that differ at least once, leaving for residuals the matrices $R_k \neq R_k'$. Since the columns of R_k and R_k' are identical up to a permutation of each pair of columns at addresses where $\mathbf{v}_k$ and $\mathbf{v}_k'$ differ, $R_k \cdot cp \cdot R_k'$.

Applying the MM-algorithm to R_k and R_k', suppose c_{k+1} and c_{k+1}' to be the coefficients extracted, respectively. $R_k \cdot cp \cdot R_k'$ implies that all column maximums in R_k and R_k' are equal, so $c_{k+1} = c_{k+1}'$. Repetition of the argument above now yields for the new residuals $R_{k+1} \cdot cp \cdot R_{k+1}'$. In view of this, identical coefficients must be extracted at every step. From which there follows (16a) and (16b). Q.E.D.

Now suppose that $\sum_{k=1}^{q} d_k W_k$ is any convex decomposition of $U \in P_{fc}$, and that $\{c_1, c_2,..., c_p\}$ are the coefficients for a MM-decomposition. Assuming without loss that the $\{d_k\}$ are monotone decreasing, $1 \geqslant d_1 \geqslant d_2 \cdots \geqslant d_q > 0$, we note that $c_1 \geqslant d_1$, because c_1 is the largest possible coefficient that can be factored from U. If $c_1 = d_1$ we may take $W_1 = U_1$ in the MM-decomposition, i.e., $W_1 = U_1 = U_{mm}$. Continuing in this fashion, we can construct from the W_k's a MM sequence as long as the d_k's continue to equal the c_k's. Either this process terminates with $p = q$ and $d_k = c_k \ \forall k$; or at some j, $d_j < c_j$. This proves

THEOREM 3. *Let $U \in P_{fc}$. The coefficient vector $\mathbf{c}_{mm} = (c_1, c_2,..., c_p)$ for all MM-decompositions of U is lexicographically larger than the coefficient vector $\mathbf{d} = (d_1, d_2,..., d_q)$ for any other convex decomposition of U.*

Since the sum of convex coefficients in every convex decomposition of U is one, it is plausible to presume that the *size* of each coefficient is a measure of the relative efficacy of its associated hard partition of X as a factor in the construction of fuzzy partition U. Theorem 3 shows that U_{mm}, the first term of every MM-decomposition of U, is always the "strongest" possible dominant term, and the remaining terms in MM-decompositions form the optimal sequence of factor partitions in the sense of coefficient magnitudes. Empirical evidence as well as one's intuition suggest that a related property of MM-decomposition is also true:

Conjecture. Let $U \in P_{fc}$. If $\sum_{k=1}^{p} c_k U_k$ is any MM-decomposition of U, and $\sum_{k=1}^{q} d_k W_k$ is any other decomposition of U, then $p \leqslant q$.

Indeed, $p = 2$ implies $q \geqslant 2$, for otherwise $q = 1$ implies $U \in P_{c0}$ so $p = 1$. At $p = 3$ the same argument shows that $q \neq 1$, so the conjecture is true unless

$q = 2$. If $q = 2$, then $c_1 + c_2 + c_3 = d_1 + d_2 = 1$. Theorem 3 insures us that $c_1 \geqslant d_1$ and $c_1 \geqslant d_2$. If c_1 were equal to either d_1 or d_2, we could choose for the corresponding W_j the matrix U_1, leaving equal residuals $U - c_1 U_1 = U - d_j W_j$. Then the remaining d_k must equal c_2, for otherwise maximality of c_2 contradicts $c_2 \geqslant d_k$, and $d_k \leqslant c_2$ implies that $1 = d_j + d_k$, $c_1 + c_2 = 1$. In either case, this leaves $c_3 = 0$ so $p \neq 3$. On the other hand, if $c_1 > d_1$ and $c_1 > d_2$, then because $c_1 = u_{ij}$ for some i and j, it is necessary that $c_1 = d_1 + d_2 = 1$, so $c_2 = c_3 = 0$, and again $p \neq 3$, thus, $p = 3$ implies $q \geqslant 3$. These remarks establish the conjecture for $p \leqslant 3$, and strongly support our guess that *MM*-decomposition is always minimal in length.

V. Reclassification Decomposition

F-decompositions force at least one residual membership to zero at each step in their application: we interpret this as forcing the individual concerned out of its membership in the class it leaves. In *MM*-decomposition all n subjects begin in their maximum membership classes (in $U_1 = U_{mm}$), and when c_2 is extracted as many individuals as possible are allowed to shift classes in the hard partition U_2. An algorithm for decomposition which is based on membership thresholding and proceeds quite differently from the *MM*-algorithm is the

Reclassification (or R) Decomposition

Let $U \in P_{fc}$. From U we first construct a ranking matrix $\rho(U) \in V_{cn}$ as follows: ρ_{ij} is the integer in $I_c = \{1, 2,..., c\}$ which gives the rank of u_{ij} in column j, $1 \leqslant j \leqslant n$, after ordering the elements of each column of U in descending order.

A second matrix $\sigma(U) \in V_{cn}$ is then derived from $\rho(U)$ by taking cumulative sums of entries in U: wherever $\rho_{ij} = 1$, define $\sigma_{ij} = u_{ij}$; where $\rho_{ij} = 2$, define $\sigma_{ij} = u_{i_1,j} + u_{ij}$, where $\rho_{i_1,j} = 1$; and so on. In other words, the entries in columns of $\sigma(U)$ are cumulative sums of the memberships of each $\mathbf{x}_k$ in the c fuzzy sets exhibited in U: the values in column j ascend from the largest memberships, and so on up to 1, the addresses of this ordered sequence being found at 1, 2,..., c in the corresponding column of $\rho(U)$. For example, with

$$U = \begin{bmatrix} .70 & .40 & .03 & .15 \\ .20 & .50 & .07 & .80 \\ .10 & .10 & .90 & .05 \end{bmatrix}, \tag{18}$$

we have

$$\rho(U) = \begin{bmatrix} 1 & 2 & 3 & 2 \\ 2 & 1 & 2 & 1 \\ 3 & 3 & 1 & 3 \end{bmatrix}; \qquad \sigma(U) = \begin{bmatrix} .70 & .90 & 1 & .95 \\ .90 & .50 & .97 & .80 \\ 1 & 1 & .90 & 1 \end{bmatrix}.$$

Next, we array the $n(c-1)$ smallest positive entries of $\sigma(U)$ in increasing order, label them a_1 to a_m, $m = n(c-1)$, define $a_0 = 0$; $a_{m+1} = 1$, and calculate their successive differences:

$$0 = a_0 < a_1 \leqslant a_2, \quad \cdots \leqslant a_m \leqslant a_{m+1} = 1 \tag{19}$$

$$c_{j+1} = a_{j+1} - a_j; \qquad 0 \leqslant j \leqslant m. \tag{20}$$

The c_j's all lie in [0, 1], and by their definition sum to 1, $\sum_{j=1}^{m+1} c_j = a_{m+1} - a_0 = 1$: these are the convex coefficients of the R-decomposition of U. Since a_1 is the smallest positive entry in $\sigma(U)$, $c_1 = a_1 - a_0$ is the minimum maximum membership in U. That is, *the first coefficient extracted by both the R and MM algorithms is always the same one — the largest possible one.* For the matrix at (18) we have from (U)

$$\begin{aligned}
a_0 &= .00 \\
a_1 &= .50 \quad > c_1 = .50 \\
a_2 &= .70 \quad > c_2 = .20 \\
a_3 &= .80 \quad > c_3 = .10 \\
a_4 &= .90 \quad > c_4 = .10 \\
a_5 &= .95 \quad > c_5 = .05 \\
a_6 &= .97 \quad > c_6 = .02 \\
a_7 &= 1 \quad\;\;\, > c_7 = .03.
\end{aligned} \tag{21}$$

Note that even though c_1 is always the largest coefficient extracted, this sequence is *not* necessarily monotone decreasing; it will be *unique* and of length $n(c-1)+1$ whenever the ordering in (19) is strict. To complete the decomposition, we define hard partitions $U_k \in P_{c0}$ corresponding to the c_k's as follows: $U_1 = U_{mm}$ is again the maximum membership matrix, and is the dominant term of both the R and MM decompositions; every $\mathbf{x}_k \in X$ belongs initially to its class of maximum membership. Now think of $r_k = \sum_{j=1}^{k} c_j$ as the *threshold* at step k in the R-algorithm; note that $t_k = a_k$ for $k > 1$. At step k locate the address (or addresses) in $\sigma(U)$ where threshold a_k occurs, and define U_k equal to U_{k-1} except: at each address where a_k occurs in $\sigma(U)$, set $(u_k)_{ij} = 0$, and move the 1's that occupied these addresses to the place where their next lowest membership occurs, i.e., to the next highest integer address in the corresponding column of ranking matrix $\rho(U)$. This transition rule amounts to reclassifying between U_i and U_j, $i < j$, all of those vectors which are thresholded from their upper to lower "halves" in $\sigma(U)$ as theshold t runs through $(t_i, t_j]$. This procedure is admittedly hard to described verbally, but should be clear from the example to follow: from (18) and (21) we would proceed by imagining threshold t to begin at 0; for $0 \leqslant t \leqslant .50$ no reclassification is made, and we have

$$c_1 U_1 = c_1 U_{mm} = .50 \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}. \tag{22}$$

As soon as t becomes greater than .50, vector $\mathbf{x}_2$ cannot tolerate membership in class 2 (one sees this by finding $t = .50$ at address (2, 2) in $\sigma(U)$); to find the destination of $\mathbf{x}_2$, go to address (2, 2) in $\rho(U)$, and find the address of the next highest integer, in this case, address (1, 2). Thus the transition from U_1 to U_2 at $t = 0.5$ is made by sending $\mathbf{x}_2$ from (2, 2) in U_1 to (1, 2) in U_2, and we have for all $t \in (.50, .70]$

$$c_2U_2 = .20 \begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}.$$

The sequence of transitions obtained in this fashion can be recorded in the matrix $\rho(U)$ with arrows and indices indicating the stage at which the transition occured. Thus we have at first in $\rho(U)$

$$\rho(U) = \begin{bmatrix} 1 & & 2 & & 3 & 2 \\ & \textcircled{2} & & \textcircled{1} & & \\ 2 & & 1 & & 2 & 1 \\ & & & & & \\ 3 & & 3 & & 1 & 3 \end{bmatrix}.$$

Increasing t above .70 results in degrading the membership of vector $\mathbf{x}_1$ from class 1 to class 2, as seen by first inspecting $\sigma(U)$ to locate the threshold, and then $\tilde{\rho}(U)$ to find the path of the transition. This second switch is shown above in $\rho(U)$. Thus for all $t \in (.70, .80]$ we have

$$c_3U_3 = .10 \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}.$$

Sequential reclassification via the R-algorithm is perhaps most easily understood when $c = 2$, for then each transition made merely moves one or more subjects from their maximum to minimum membership classes. To exemplify further, we rework the example of Section IV using the R-decomposition for matrix U shown at (13):

$$U = \begin{bmatrix} .90 & .80 & .30 & .40 & .05 \\ .10 & .20 & .70 & .60 & .95 \end{bmatrix}. \tag{13}$$

From U we find that

$$\rho(U) = \begin{bmatrix} 1 & 1 & 2 & 2 & 2 \\ 2 & 2 & 1 & 1 & 1 \end{bmatrix};$$

$$\sigma(U) = \begin{bmatrix} .90 & .80 & 1 & 1 & 1 \\ 1 & 1 & .70 & .60 & .95 \end{bmatrix};$$

$$\begin{aligned} a_0 &= .00 \\ &\quad > c_1 = .60 \\ a_1 &= .60 \\ &\quad > c_2 = .10 \\ a_2 &= .70 \\ &\quad > c_3 = .10 \\ a_3 &= .80 \\ &\quad > c_4 = .10 \\ a_4 &= .90 \\ &\quad > c_5 = .05 \\ a_5 &= .95 \\ &\quad > c_6 = .05. \\ a_6 &= 1 \end{aligned}$$

To begin, we have from above that

$$c_1 U_1 = .60 \begin{bmatrix} 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 \end{bmatrix},$$

with residual

$$R_1 = \begin{bmatrix} .30 & .20 & .30 & .40 & .05 \\ .10 & .20 & .10 & 0 & .35 \end{bmatrix}.$$

While in a general decomposition the next coefficient $c_2 = .10$ could be extracted in many ways, the R-algorithm proceeds by degrading the vector whose membership in its maximum membership class is first exceeded upon crossing the threshold $t = 0.60$; in this case, from $\sigma(U)$ we find at address (2, 4) that $\mathbf{x}_4$ has the lowest tolerance, and must be reclassified (to address (1, 4) here) first:

$$c_2 U_2 = .10 \begin{bmatrix} 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \end{bmatrix}.$$

Increasing t above .70 results in degrading the membership of $\mathbf{x}_3$

$$c_3 U_3 = .10 \begin{bmatrix} 1 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

At $t > .80$, $\sigma_{12} = .80 \Rightarrow$ reclassify $\mathbf{x}_2$:

$$c_4 U_4 = .10 \begin{bmatrix} 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 \end{bmatrix}.$$

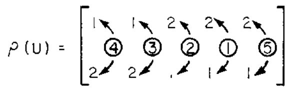
At $t < .90$, $\sigma_{11} = .90 \Rightarrow$ reclassify $\mathbf{x}_1$:

$$c_5 U_5 = .05 \begin{bmatrix} 0 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 & 1 \end{bmatrix}.$$

Finally, for $t > .95$, $\sigma_{25} = .95$ requires us to reclassify $\mathbf{x}_5$ last; this is due to its most distinctive memberships in U:

$$c_6 U_6 = .05 \begin{bmatrix} 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 \end{bmatrix}.$$

The entire sequence of transitions for this example may be recorded in the matrix $\rho(U)$ as follows:



From this we see that the sequence of transitions always proceeds "uphill" through the ranked columns of $\rho(U)$, from $1 \to 2 \cdots \to c$. Note that U_1 and the final partition U_6 are algebraic complements; it is *always* the case that the first and last partitions in an R-decomposition sequence are the maximum and minimum membership partitions which are the closest and farthest hard partitons associated with U respectively. Since the $\{a_k\}$ were strictly ordered in this example, the R-decomposition was unique.

Since the first (and dominant) term of every R and MM decomposition is U_{mm}, one might conjecture that U_{mm} is the dominant term in every convex decomposition of $U \in P_{fc}$. To see that this is *not* the case, consider the matrix

$$U = \begin{bmatrix} .54 & .58 & .73 & .56 \\ .46 & .42 & .27 & .44 \end{bmatrix}, \tag{23}$$

with maximum membership matrix $U_{mm} = \left[\begin{smallmatrix} 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 \end{smallmatrix}\right]$. We exhibit for this U the MM-decomposition, and a second convex decomposition which not only does not have U_{mm} in it, but is in fact, entirely disjoint in the sense that no hard partition used in the MM-decomposition is used in the second one:

MM–decomposition of (23)	Another disjoint decomposition
$+ .54 \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix}$	$+ .44 \begin{bmatrix} 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$
$+ .27 \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix}$	$+ .29 \begin{bmatrix} 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \end{bmatrix}$
$+ .15 \begin{bmatrix} 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \end{bmatrix}$	$+ .13 \begin{bmatrix} 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix}$
$+ .02 \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \end{bmatrix}$	$+ .10 \begin{bmatrix} 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
$.02 \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}.$	$+ .04 \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix}.$

Although the term U_{mm} which dominates both the MM and R decompositions does not always appear, it carries the coefficient c_1 which is maximum among all possible coefficients for a given U; accordingly, we presume that the equivalence relation induced on $X \times X$ by U_{mm} indicates the maximal strength of bonding at level c_1 which the vectors in X enjoy when partitioned by U. A forthcoming paper will deal at length with the relationships between fuzzy partitions and fuzzy similarity relations in $X \times X$.

Finally, we observe that sequential application of the R algorithm to its residuals at each step results in a MM-decomposition of U.

VI. Convex Decomposition and the Partition Coefficient

For $U \in V_{cn}$ the Euclidean matrix norm and and inner product from which it is derived are

$$\| U \| = (\mathrm{tr}(UU^t))^{1/2} \tag{24a}$$

$$\langle U, U \rangle = \mathrm{tr}(UU^t) = \| U \|^2 \tag{24b}$$

where $\mathrm{tr}(\cdot)$, $(\cdot)^t$ respectively denote the trace and transpose operations. Following [5] we denote by F: $V_{cn} \to R$ the function

$$F(U) = \frac{\| U \|^2}{n}. \tag{25}$$

Since $F(U)$ is inversely proportional to the overall content of pairwise fuzzy intersections in U, it has been called the *partition coefficient of* U. It measures the overall "fuzziness" in U via the following results proven in [5]:

$$1/c \leqslant F(U) \leqslant 1 \ \forall \ U \in P_{fc}, \tag{26a}$$

$$1/c = F(\tilde{U}) \Leftrightarrow \tilde{U} = [1/c], \tag{26b}$$

$$1 = F(U) \Leftrightarrow U \in P_{c0} \text{ is hard.} \tag{26c}$$

If we denote by $d(U, V) = \| U - V \|$ the distance between U and V in V_{cn}, it is easy to check that $d(U, \tilde{U}) = (n(c-1)/c)^{1/2} \ \forall \ U \in P_{c0}$; consequently, the matrix $\tilde{U}$ is the geometric centroid of P_{fc}. Loosely speaking, $\tilde{U}$ is the fuzziest classification of the vectors in X allowed in P_{fc}, whereas $U's \in P_{c0}$ are the crispest (hardest).

Now suppose U_i and U_j are any pair of hard c-partitons of X. We shall write $U_i \leftrightarrow U_j$ to indicate that U_i and U_j are different classification states for X that can be realized from each other by a finite number n_{ij} of transitions (or reclassifications) between stages i and j. For example, if

$$U_i = \begin{bmatrix} 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 \end{bmatrix} \quad \text{and} \quad U_j = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \end{bmatrix}, \tag{27}$$

then $n_{ij} = 2$ for $U_i \leftrightarrow U_j$. It is quite useful for our later work to note that n_{ij} can be calculated readily as

$$n_{ij} = n - \operatorname{tr}(U_i U_j^t). \tag{28}$$

To see this, consider number

$$N_{ij} = \operatorname{tr}(U_i U_j^t) = \sum_{k=1}^{c} \sum_{t=1}^{n} (u_i)_{kt} (u_j)_{kt} . \tag{29}$$

Since $(u_i)_{kt}$ and $(u_j)_{kt}$ are respectively the membership of $\mathbf{x}_t$ in the k-th cluster of U_i and U_j, each term in the sum at (29) is 1 iff $\mathbf{x}_t$ is *not* reclassified in the transition $U_i \leftrightarrow U_j$. Thus N_{ij} is the total number of individuals not reclassified, and hence $n_{ij} = n - N_{ij}$ at (28) is the number which are reclassified, and

$$f_{ij} = \frac{n_{ij}}{n} = \frac{n - N_{ij}}{n} \tag{30}$$

is the faction or percent of individuals reclassified during $U_i \leftrightarrow U_j$. For instance, we have for the matrices in (27) $n_{ij} = 2$, $N_{ij} = 3$, and $f_{ij} = \frac{2}{5} = .40$, i.e., 40% of the data is reclassified.

The following theorem exhibits the relationship between the partition coefficient $F(U)$ and the amount of reclassification done in the terms of any convex decomposition of U:

THEOREM 4. *Let $U \in P_{fc}$, $F(U)$ as in* (25), *f_{ij} as in* (29), *and suppose that $U = \sum_{k=1}^{p} c_k U_k$ is any convex decomposition of U. Then*

$$F(U) = 1 - \sum_{j=j+1}^{p} \sum_{i=1}^{p-1} c_i f_{ij} c_j . \tag{30}$$

Proof.

$$F(U) = F\left(\sum_{k=1}^{p} c_k U_k\right) = (1/n)\left(\operatorname{tr}\left(\sum_{j=1}^{p} c_j U_j\right)\left(\sum_{j=1}^{p} c_j U_j\right)^t\right)$$

$$= (1/n)\left(\operatorname{tr}\left(\sum_{j=1}^{p} \sum_{i=1}^{p} c_i U_i U_j^t c_j\right)\right)$$

$$= (1/n)\left(\sum_{j=1}^{p} \sum_{i=1}^{p} c_i \operatorname{tr}(U_i U_j^t)\, c_j\right)$$

$$= \sum_{j=1}^{p} \sum_{i=1}^{p} c_i (N_{ij}/n)\, c_j .$$

Observing that $N_{ij} = N_{ji} \forall i \neq j$, and that $N_{ii} = nF(U_i) = n \forall i$, we have

$$F(U) = \sum_{j=1}^{p} c_j(N_{jj}/n) c_j + 2\left(\sum_{j=i+1}^{p} \sum_{i=1}^{p-1} c_i(N_{ij}/n) c_j\right)$$

$$= \sum_{j=1}^{p} c_j^2 + 2\left(\sum_{j=i+1}^{p} \sum_{i=1}^{p-1} c_i((n - (n - N_{ij}))/n) c_j\right)$$

$$= \left\{\sum_{j=1}^{p} c_j^2 + 2\left(\sum_{j=i+1}^{p} \sum_{i=1}^{p-1} c_i c_j\right)\right\} - 2\left(\sum_{j=i+1}^{p} \sum_{i=1}^{p-1} c_i f_{ij} c_j\right)$$

$$= 1 - 2\left(\sum_{j=i+1}^{p} \sum_{i=1}^{p-1} c_i f_{ij} c_j\right),$$

the last equality following because the c_j are convex coefficients, so they sum to 1. Q.E.D.

Equation (30) shows that $F(U) = 1$ iff $f_{ij} = 0 \forall i \neq j$ iff $n = N_{ij} \forall i \neq j$ iff no point is ever reclassified in any convex decomposition of U iff $U \in P_{c0}$ is hard and is its own unique convex decomposition, $p = c_1 = 1$. An equivalent way to state Theorem 4 as as follows; we define the $p \times p$ *transition matrix*

$$N = \left[\frac{N_{ij}}{n}\right]; \qquad N_{ij} = \operatorname{tr}(U_i U_j^t); \qquad 1 \leq i, \quad j \leq p. \tag{31}$$

Matrix N is symmetric and positive-definite for $U \in P_{c0}$, and may thus be used to induce the weighted inner product $\langle \mathbf{c}, \mathbf{c} \rangle_N = \|\mathbf{c}\|_N^2 = \mathbf{c}^t N \mathbf{c}$ on $\mathbb{R}^p$. Using this notation, we have from the proof of Theorem 4 the

COROLLARY. *Let $U \in P_{fc}$, and suppose $U = \sum_{k=1}^{p} c_k U_k = \sum_{k=1}^{q} c_k' U_k'$ are two convex decompositions of U. Let N and N' be their respective transition matrices computed via* (31), *and let* $\mathbf{c}$ *and* $\mathbf{c}'$ *be their vectors of convex coefficients in $\mathbb{R}^p$ and $\mathbb{R}^q$. Then*

$$\|\mathbf{c}\|_N = \|\mathbf{c}'\|_{N'}. \tag{32}$$

Proof. Expansion of U in any decomposition leads to, for example, $F(U) = \sum_{j=1}^{p} \sum_{i=1}^{p} (c_i N_{ij} c_j/n) = \mathbf{c}^t N \mathbf{c} = \|\mathbf{c}\|_N^2$. Since $F(U)$ is fixed, (32) follows. Q.E.D.

The implication of (32) is this; all convex decompositions of U are equivalent in the sense that their vectors of convex coefficients have equal lengths when normalized by the amount of reclassification required by their respective sequences of hard transitions. Since the ij-th entry of N is the fraction of individuals *not* reclassified in the transition $U_i \leftrightarrow U_j$, the value $F(U) = \mathbf{c}^t N \mathbf{c}$ maximizes (for different partitions U) when the overall amount of reclassification is minimized: this is a new justification for the clustering strategy of maximizing F outlined in [5]. Evidently the quadratic form $\mathbf{c}^t N \mathbf{c}$ increases as the number of "stable" points in the data does, maximizing when no reclassification is necessary.

Assuming without loss that U_i and U_j are distinct, it will be seen that N_{ij}/n is always less than 1 for $i \neq j$. We emphasize here that this is the number or fraction of vectors not reclassified in the *single-step* transition $U_i \leftrightarrow U_j$, even though U_i and U_j may be actually realized via a multi-step transition which would accumulate a different fraction of fixed addresses. For example, the transition shown in (27) has $N_{ij}/n = 3/5 = .6$, so 60% of the data is stable during the transition. We could, however, realize U_j from U_i in the two-step transition

$$U_i = \begin{bmatrix} 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 \end{bmatrix} \leftrightarrow U_k = \begin{bmatrix} 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 \end{bmatrix} \leftrightarrow U_j = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \end{bmatrix}. \tag{33}$$

In (33) we have $N_{ik}/n = 0/5 = .00$; $N_{kj}/n = 2/5 = .40$; and $N_{ij}/n = .60$ as above. Thus $U_i \leftrightarrow U_j \leftrightarrow U_k$ but $N_{ij} \neq N_{ik} + N_{kj}$.

To solidify these ideas we decompose the matrix at (34) with both the MM and R algorithms:

$$U = \begin{bmatrix} .39 & .60 & .35 & .17 & .92 \\ .17 & .14 & .37 & .78 & .05 \\ .44 & .26 & .28 & .05 & .03 \end{bmatrix} \doteq R_0. \tag{34}$$

(i) *MM-decomposition of* (34). The initial MM path is $\mathbf{v}_1 = (*_{31}, *_{12}, *_{23}, *_{24}, *_{15})$, with minimum maximum membership $c_1 = u_{23} = .37$,

$$c_1U_1 = .37 \begin{bmatrix} 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix}; \qquad R_1 = \begin{bmatrix} .39 & .23 & .35 & .17 & .55 \\ .17 & .14 & .00 & .41 & .05 \\ .07 & .26 & .28 & .05 & .03 \end{bmatrix}.$$

From $\mathbf{v}_2 = (*_{11}, *_{32}, *_{13}, *_{24}, *_{15})$ we infer that $c_2 = (r_1)_{32} = .26$, so

$$c_2U_2 = .26 \begin{bmatrix} 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{bmatrix}; \qquad R_2 = \begin{bmatrix} .13 & .23 & .09 & .17 & .29 \\ .17 & .14 & .00 & .15 & .05 \\ .07 & .00 & .28 & .05 & .03 \end{bmatrix}$$

$\mathbf{v}_3 = (*_{21}, *_{12}, *_{33}, *_{14}, *_{15}) \Rightarrow c_3 = (r_2)_{21} = (r_2)_{14} = .17$, from which

$$c_3U_3 = .17 \begin{bmatrix} 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{bmatrix}; \qquad R_3 = \begin{bmatrix} .13 & .06 & .09 & .00 & .12 \\ .00 & .14 & .00 & .15 & .05 \\ .07 & .00 & .11 & .05 & .03 \end{bmatrix}$$

$\mathbf{v}_4 = (*_{11}, *_{22}, *_{33}, *_{24}, *_{15}) \Rightarrow c_4 = (r_3)_{33} = .11$, leading to

$$c_4U_4 = .11 \begin{bmatrix} 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{bmatrix}; \qquad R_4 = \begin{bmatrix} .02 & .06 & .09 & .00 & .01 \\ .00 & .03 & .00 & .04 & .05 \\ .07 & .00 & .00 & .05 & .03 \end{bmatrix}$$

$\mathbf{v}_5 = (*_{31}, *_{12}, *_{13}, *_{34}, *_{25}) \Rightarrow c_5 = (r_4)_{34} = (r_4)_{25} = .05$, yielding

$$c_5U_5 = .05 \begin{bmatrix} 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \end{bmatrix}; \qquad R_5 = \begin{bmatrix} .02 & .01 & .04 & .00 & .01 \\ .00 & .03 & .00 & .04 & .00 \\ .02 & .00 & .00 & .00 & .03 \end{bmatrix}.$$

At step 6 we encounter with MM-decomposition the first non-unique path of minimum maximum menbership in R_5 because of the tie in its first column. Choosing the upper path leads to $\mathbf{v}_6 = (*_{11}, *_{22}, *_{13}, *_{24}, *_{35})$ and the choice $c_6 = (r_5)_{11} = .02$, whence

$$c_6U_6 = .02 \begin{bmatrix} 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}; \qquad R_6 = \begin{bmatrix} .00 & .01 & .02 & .00 & .01 \\ .00 & .01 & .00 & .02 & .00 \\ .02 & .00 & .00 & .00 & .01 \end{bmatrix}.$$

In the seventh step there are four MM paths in R_6. For the choice $\mathbf{v}_7 = (*_{31}, *_{12}, *_{13}, *_{24}, *_{15})$, $c_7 = (r_6)_{12} = (r_6)_{15}$ gives

$$c_7U_7 = .01 \begin{bmatrix} 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix}; \qquad R_7 = \begin{bmatrix} .00 & .00 & .01 & .00 & .00 \\ .00 & .01 & .00 & .01 & .00 \\ .01 & .00 & .00 & .00 & .01 \end{bmatrix}$$

and from R_7 we have at the last stage of MM-decomposition

$$c_8U_8 = .01 \begin{bmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \end{bmatrix};$$

with $R_8 = \theta$, the zero matrix.

(ii) *R-Decomposition of* (34). This decomposition begins with the construction of the ranking and cumulative sum matrices $\rho(U)$ and $\sigma(U)$. Repeating (34) for convenience, we have

$$U = \begin{bmatrix} .39 & .60 & .35 & .17 & .92 \\ .17 & .14 & .37 & .78 & .05 \\ .44 & .26 & .28 & .05 & .03 \end{bmatrix};$$

$$\rho(U) = \begin{bmatrix} 2 & 1 & 2 & 2 & 1 \\ 3 & 3 & 1 & 1 & 2 \\ 1 & 2 & 3 & 3 & 3 \end{bmatrix};$$

$$\sigma(U) = \begin{bmatrix} .83 & .60 & .72 & .95 & .92 \\ 1 & 1 & .37 & .78 & .97 \\ .44 & .86 & 1 & 1 & 1 \end{bmatrix}.$$

From $\sigma(U)$ we array the thresholds $\{a_k\}$ and from them derive the successive differences, say $\{d_k\}$:

$$\begin{array}{ll} a_0 = .00 & \\ & > d_1 = .37 \\ a_1 = .37 & \\ & > d_2 = .07 \\ a_2 = .44 & \\ & > d_3 = .16 \\ a_3 = .60 & \\ & > d_4 = .12 \\ a_4 = .72 & \\ & > d_5 = .06 \\ a_5 = .78 & \\ & > d_6 = .05 \\ a_6 = .83 & \\ & > d_7 = .03 \\ a_7 = .86 & \\ & > d_8 = .06 \\ a_8 = .92 & \\ & > d_9 = .03 \\ a_9 = .95 & \\ & > d_{10} = .02 \\ a_{10} = .97 & \\ & > d_{11} = .03. \\ a_{11} = 1 & \end{array}$$

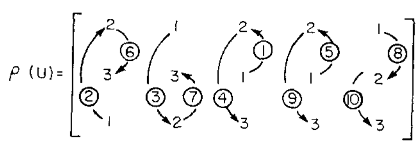
Using $\sum d_k W_k$ for the form of the R-decomposition, the initial term $d_1 W_1$ is exactly the same as $c_1 U_1$ in the MM-decomposition above, with identical residual. Upgrading the threshold from .00, all data points are stable until $t > .37$, at which time $\mathbf{x}_3$ must be transferred from class 2 to class 1 (from $\sigma(U)$ we see that $\mathbf{x}_3$ will now remain in class 1 until $t > .72$, at which time it will transfer from class 1 to class 3). Reclassifying $\mathbf{x}_3$ results in the second term

$$d_2 W_2 = .07 \begin{bmatrix} 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix}; \qquad R_2 = \begin{bmatrix} .39 & .16 & .28 & .17 & .48 \\ .17 & .14 & .00 & .34 & .05 \\ .00 & .26 & .28 & .05 & .03 \end{bmatrix}.$$

The threshold is now increased without change in classification until it crosses the next cumulative sum, $t > .44$. At this stage $\mathbf{x}_1$ becomes unstable in class 3 and must be transferred to class 1, where it will remain until $t > .83$;

$$d_3 W_3 = .16 \begin{bmatrix} 1 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}; \qquad R_3 = \begin{bmatrix} .23 & .00 & .12 & .17 & .32 \\ .17 & .14 & .00 & .18 & .05 \\ .00 & .26 & .28 & .05 & .03 \end{bmatrix}.$$

Since the ordering of the $\{a_k\}$ was strict, we expect a unique 11 term R-decomposition of U. To shorten this example we record the unique sequence of reclassifications as address transfers in the matrix $\rho(U)$:



The sequence of transitions recorded in $\rho(U)$ indicates the stability of each of the W_k's to cumulative membership thresholding. The sequence suggests that $\mathbf{x}_3$ is the least stable or most undistinctive data point, since it is transferred twice in the early stages of decomposition, whereas $\mathbf{x}_5$ holds its initial classification the longest, indicating its relative certainty of membership distribution in the given fuzzy partition.

The partition coefficient $F(U)$ for this U is $F(U) = \mathbf{c}^t N \mathbf{c} = \mathbf{d}^t N' \mathbf{d} = \operatorname{tr}(UU^t)/n = .53$, where

$$\mathbf{c}^t = (.37, .26, .17, .11, .05, .02, .01, .01)$$

$$\mathbf{d}^t = (.37, .07, .16, .12, .06, .05, .03, .06, .03, .02, .03)$$

and N, N' are the 8×8 and 11×11 transition matrices calculated via (31) for the MM and R decompositions respectively. Since $c = 3$ we know that $.33 \leqslant F(U) \leqslant 1$: accordingly, .53 is a relatively low partition coefficient, indicating a fuzzy partition containing quite a bit of fuzzy uncertainty. This is manifested in the convex decompositions by coefficients which have no strongly dominant term. Thus $c_1 U_1 = d_1 W_1 = .37 U_{mm}$ indicates a relatively low minimum maximum membership bonding for the relation induced on the data by U_{mm}; indeed, for $c = 3$ the weakest possible dominant term has for its coefficient .33, so that one's confidence (of .37) in taking U_{mm} as a first approximation to hard clusters in X should be slight.

VII. Summary

Several important facts about convex decompositions of fuzzy c-partitions of X have been enumerated. In particular, the dimension of fuzzy c-partition space is $n(c - 1)$. Two algorithms for decomposition have been analyzed and exemplified. Both of these algorithms are rather tedious to work with by hand, but are quite readily programmed for large scale problems involving real data sets. The relationship between convex decomposition and the partition coefficient provides additional justification for a previously advocated fuzzy clustering strategy. The authors plan to devote a forthcoming paper to the connection between fuzzy partition spaces and fuzzy similarity relation spaces, in which analogs of the convex decompositions described above will hopefully lead to a new method for clustering with fuzzy graphs.

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