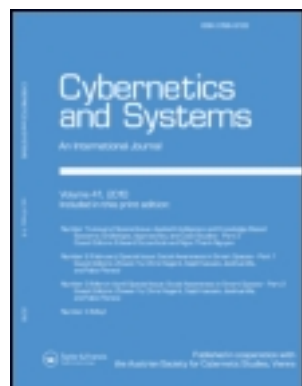


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Publisher: Taylor & Francis

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Journal of Cybernetics

Publication details, including instructions for authors and subscription information:

<http://www.tandfonline.com/loi/ucbs19>

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Published online: 30 Apr 2008.

To cite this article: J. C. Dunnt (1974): Well-Separated Clusters and Optimal Fuzzy Partitions, Journal of Cybernetics, 4:1, 95-104

To link to this article: <http://dx.doi.org/10.1080/01969727408546059>

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Well-Separated Clusters and Optimal Fuzzy Partitions

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Abstract

Two separation indices are considered for partitions $P = \{X_1, \dots, X_k\}$ of a finite data set X in a general inner product space. Both indices increase as the pairwise distances between the subsets X_i become large compared to the diameters of X_i . Maximally separated partitions P^* are defined and it is shown that as the indices of P^* increase without bound, the characteristic functions of X_i^* in P^* are approximated more and more closely by the membership functions in fuzzy partitions which minimize certain fuzzy extensions of the k -means squared error criterion function.

1. Introduction

In reference [1], the problem of detecting the presence or absence of compact well separated (CWS) clusters in a large finite data set X was approached by considering a related extremization problem for fuzzy extensions of the standard k -means squared error criterion function. When k CWS clusters $\{X_1, \dots, X_k\}$ are present in X it is plausible that the membership functions in a globally minimizing fuzzy partition should approximate the characteristic functions of the clusters X_i more and more closely as the separation between clusters increases. On the other hand, when well-separated clusters are not present in X , one expects the minimizing fuzzy partition to consist of membership functions which are truly fuzzy in the sense that their values differ substantially from 0 or 1 over certain regions in X . These conjectures were supported by a number of specific examples described in [1], however no formal proofs were available at that time. In this paper, we formulate a precise statement and rigorous proof of the first conjecture.

2. Separation Indices

Let X denote a finite subset of a general real inner product space V , i.e., a real vector space equipped with a symmetric positive definite bi-linear real function, $\langle u|v \rangle$ defined for all pairs of vectors u, v in V [2]. The inner product $\langle u|v \rangle$ induces a metric d on V according to

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the rule,

$$d(u, v) \triangleq \|u - v\| \triangleq \langle u - v | u - v \rangle^{1/2}$$

With respect to this distance we may define diameters of subsets of X and distances between subsets of X in the standard fashion, namely,

$$\begin{aligned} \text{diam } A &\triangleq \max_{x, y \in A} d(x, y) \\ \text{dist}(A, B) &\triangleq \min_{\substack{x \in A \\ y \in B}} d(x, y) \end{aligned}$$

where $A, B \subset X$ and $A, B \neq \phi$ (empty set).

A k -partition of X is any family $P = \{X_1, \dots, X_k\}$ of k non empty, mutually disjoint, and exhaustive subsets of X , i.e.

$$\begin{aligned} X_i &\neq \phi \quad 1 \leq i \leq k \\ X_i \cap X_j &= \phi \quad i \neq j \\ \bigcup_{i=1}^k X_i &= X \end{aligned} \tag{1}$$

The class of all such partitions is denoted by $\mathcal{P}(k)$. To each k -partition P we attach a separation index $\alpha(k, P)$ defined by the rule

$$\alpha(k, P) = \min_{1 \leq q \leq k} \min_{\substack{1 \leq r \leq k \\ r \neq q}} \text{dist}(X_q, X_r) / \max_{1 \leq p \leq k} \text{diam}(X_p) \tag{2}$$

and we then say that P consists of *compact separated (CS) clusters* relative to d if and only if,

$$\alpha(k, P) > 1.$$

If we put

$$\bar{\alpha}(k) = \max_P \alpha(k, P)$$

then it follows that X can be partitioned into k CS clusters if and only if

$$\bar{\alpha}(k) > 1.$$

The following result shows that X can be partitioned into k CS clusters *in at most one way*.

Theorem 1. There is at most one k -partition P of X for which $\alpha(k, P) > 1$.

Proof. Let $P^A = \{X_1^A, \dots, X_k^A\}$ and $P^B = \{X_1^B, \dots, X_k^B\}$ denote two arbitrary distinct k -partitions of X . Then at least one subset in P^A , say X_q^A , overlaps two (or more)

distinct subsets of P^B , say X_m^B and X_n^B . It follows that

$$\text{diam } X_q^A \geq \text{dist}(X_m^B, X_n^B)$$

consequently,

$$\max_{1 \leq p \leq k} \text{diam } X_p^A \geq \min_{1 \leq q \leq k} \min_{\substack{1 \leq r \leq k \\ r \neq q}} \text{dist}(X_q^B, X_r^B) \quad (3)$$

In exactly the same way we obtain

$$\max_{1 \leq p \leq k} \text{diam}(X_p^B) \geq \min_{1 \leq q \leq k} \min_{\substack{1 \leq r \leq k \\ r \neq q}} \text{dist}(X_q^A, X_r^A) \quad (4)$$

In view of (3) and (4) we therefore have

$$\frac{1}{\alpha(k, P_A)} \geq \alpha(k, P_B)$$

Thus,

$$\alpha(k, P_A) > 1 \Rightarrow \alpha(k, P_B) < 1$$

Since P_B is arbitrary, we conclude that there is at most one P such that $\alpha(k, P) > 1$.

(Q.E.D.)

In general, any partition P' in $\mathcal{P}(k)$ which satisfies,

$$\alpha(k, P') = \bar{\alpha}(k)$$

will be called a maximally separated k -partition of X , relative to the index α . In view of Theorem 1 there is precisely one maximally separated partition P' when $\bar{\alpha} > 1$.

A somewhat more demanding separation index β is obtained if the subsets X_r appearing in (2) are replaced by their convex hulls $\text{Co}X_r$ (= smallest closed convex subset of V containing X_r), i.e.,

$$\beta(k, P) = \min_{1 \leq q \leq k} \min_{\substack{1 \leq r \leq k \\ r \neq q}} \text{dist}(X_q, \text{Co}X_r) / \max_{1 \leq p \leq k} \text{diam}(X_p) \quad (5)$$

The relationship between α and β is established in the following.

Theorem 2. For all P in $\mathcal{P}(k)$,

$$\alpha(k, P) \geq \beta(k, P) \geq \alpha(k, P) - 1 \quad (6)$$

Proof. Since $\text{Co}X_r \supset X_r$, it follows that $\text{dist}(X_q, X_r) \geq \text{dist}(X_q, \text{Co}X_r)$, consequently $\alpha(k, P) \geq \beta(k, P)$.

To establish the right side of the inequality (6), we first note that every element y in the convex hull of $X_r \subset X$ is a convex combination of the elements of X_r , i.e.,

$$y = \sum_{\xi \in X_r} \sigma_\xi \cdot \xi$$

for some (finite) set of real numbers σ_ξ satisfying

$$0 \leq \sigma_\xi \leq 1 \quad \text{all} \quad \xi \in X_r$$

$$\sum_{\xi \in X_r} \sigma_\xi = 1.$$

If x, y are arbitrary elements in X_r and $\text{Co}X_r$ respectively, we then have

$$\begin{aligned} d(x, y) &= \|x - y\| \\ &= \left\| x - \sum_{\xi \in X_r} \sigma_\xi \xi \right\| \\ &= \left\| \sum_{\xi \in X_r} \sigma_\xi (x - \xi) \right\| \\ &\leq \left(\sum_{\xi \in X_r} \sigma_\xi \right) \text{diam}(X_r) = \text{diam } X_r \end{aligned} \tag{7}$$

Now, if z is any element of X_q with $q \neq r$, the triangle inequality for d gives

$$d(x, y) + d(y, z) \geq d(x, z)$$

or

$$d(y, z) \geq d(x, z) - d(x, y)$$

In view of (7) we therefore have

$$\begin{aligned} d(y, z) &\geq d(x, z) - \text{diam}(X_r) \\ &\geq d(x, z) - \max_{1 \leq p \leq k} \text{diam}(X_p) \end{aligned} \tag{8}$$

Since x, y, z are arbitrary elements of $X_r, \text{Co}X_r$, and X_q respectively it follows from (8) that

$$\text{dist}(X_q, \text{Co}X_r) \geq \text{dist}(X_q, X_r) - \max_{1 \leq p \leq k} \text{diam}(X_p)$$

Consequently,

$$\min_{1 \leq q \leq k} \min_{\substack{1 \leq r \leq k \\ r \neq q}} \text{dist}(X_q, CoX_r) \geq \min_{1 \leq q \leq k} \min_{\substack{1 \leq r \leq k \\ r \neq q}} \text{dist}(X_q, X_r) - \max_{1 \leq p \leq k} \text{diam}(X_p)$$

and therefore

$$\beta(k, P) \geq \alpha(k, P) - 1. \quad (\text{Q.E.D.})$$

The parameter β was introduced in [1], principally because of its explicit connection with fixed points of the clustering algorithm known as ISODATA. This algorithm generates partitions which are local extrema for the standard k -means least squared error criterion function, and it was shown in [1] that $\beta(k, P) > 1$ implies that P is a fixed point of the ISODATA process. The distinction between α and β is most significant when $\alpha \approx 1$, viz a vis the relationship between maximally separated partitions of X and partitions which minimize the squared error criterion or the fuzzy extensions of this criterion considered in the next section. This distinction becomes less and less important as β increases beyond 1. From Theorem 2, we can see at once that α is large compared to 1 if and only if β is large compared to 1. Furthermore, since $\beta(k, P) > 1$ implies that $\alpha(k, P) > 1$ it follows from Theorem 1 that there is at most one partition P for which $\beta(k, P) > 1$. In fact, if we put

$$\bar{\beta}(k) = \max_{P \in \Phi(k)} \beta(k, P)$$

and say that P' is maximally separated relative to β if and only if

$$\beta(k, P') = \bar{\beta}(k)$$

then it follows readily from Theorems 1 and 2 that there is precisely one maximally separated partition P' relative to β when $\bar{\beta} > 1$ and that this partition P' is also maximally separated relative to α , i.e., $\alpha(k, P') = \bar{\alpha}(k)$. Since $\bar{\alpha} > 2$ implies that $\bar{\beta} > 1$, we can now see that the distinction between CS and CWS clusters is useful only when $2 \geq \alpha > 1$ and $1 \geq \bar{\beta}$.

3. Optimal Fuzzy Partitions and Maximally Separated Partitions

Let $u_i(\cdot): X \rightarrow \{0, 1\}$ denote the characteristic function of the i^{th} subset X_i in a k -partition P , i.e.,

$$u_i(x) = \begin{cases} 0 & ; x \notin X_i \\ 1 & ; x \in X_i \end{cases}$$

and let $u(\cdot)$ denote the vector valued function $\{u_1(\cdot), \dots, u_k(\cdot)\}$. In view of (1), $u(\cdot)$ satisfies

$$\text{i) } u_i(\cdot) \not\equiv 0$$

$$\text{ii) } u_i(x) = 0 \text{ or } 1 \text{ for all } x \text{ in } X$$

$$\text{iii) } \sum_{i=1}^k u_i(x) = 1 \quad \text{for all } x \text{ in } X \quad (9)$$

Conversely, any vector valued function $u(\cdot) = \{u_1(\cdot), \dots, u_k(\cdot)\}$ which satisfies condition (9) describes a k -partition of X , viz., the partition whose subsets X_i have $u_i(\cdot)$ as their characteristic functions. Accordingly, we will denote the class of all functions $u(\cdot)$ satisfying (9) by the same symbol $\mathcal{P}(k)$ used previously to denote the class of all k -partitions of X . With this understanding, the standard k -means least squared error partitioning problem can be stated in this way: if \mathcal{L} denotes the smallest linear subspace of V containing X and \mathcal{L}^k denotes the set of all k -tuples $v = \{v_1, \dots, v_k\}$ from \mathcal{L} , find a $u'(\cdot)$ in $\mathcal{P}(k)$ and a v' in \mathcal{L}^k such that

$$\text{a. } J(u'(\cdot), v') = \min_{u(\cdot) \in \mathcal{P}(k)} \min_k J(u(\cdot), v) \quad (10)$$

where

$$\text{b. } J(u(\cdot), v) \triangleq \sum_{i=1}^k \sum_{x \in X} u_i(x) \|x - v_i\|^2 = \sum_{i=1}^k \sum_{x \in X} u_i(x) \langle x - v_i | x - v_i \rangle$$

For reasons discussed at length in [1] there are inherent advantages in considering various fuzzy extensions of the foregoing k -means partitioning problem. An infinite variety of smooth extensions of this kind are possible. For example, let $\mathcal{P}_f(k)$ denote the class of all fuzzy partitions of X , i.e., all functions $u(\cdot) = \{u_1(\cdot), \dots, u_k(\cdot)\}$ which satisfy

$$\begin{aligned} \text{i) } & u_i(\cdot) \neq 0 \\ \text{ii) } & 0 \leq u_i(x) \leq 1 \quad \text{for all } x \text{ in } X \\ \text{iii) } & \sum u_i(x) = 1 \quad \text{for all } x \text{ in } X \end{aligned} \quad (11)$$

Then for any real number $\omega \geq 1$,

$$J_\omega(u(\cdot), v) = \sum_{i=1}^k \sum_{x \in X} (u_i(x))^\omega \|x - v_i\|^2 \quad (12)$$

defines a continuous and differentiable extension of J from $\mathcal{P}(k) \times \mathcal{L}^k$ to $\mathcal{P}_f(k) \times \mathcal{L}^k$. For all such extensions it is plausible that when $\bar{\alpha}$ is sufficiently large, the component membership functions in an optimal fuzzy partition, $u'(\cdot)$, satisfying

$$J_\omega(u'(\cdot), v') = \min_{u(\cdot) \in \mathcal{P}_f(k)} \min_k J_\omega(u(\cdot), v) \quad (13)$$

should closely approximate the characteristic functions of the subsets X'_i in the maximally separated partition P' solving,

$$\alpha(k, P') = \bar{\alpha}(k).$$

Furthermore, when $\alpha \approx 1$ or smaller it is plausible that the values of the optimal membership functions $u'_i(\cdot)$ may depart significantly from the hard limits 0 or 1 over certain regions of X . Several examples substantiating the first conjecture were given in [1] for the cases $\omega = 1$ and 2, and the second conjecture for $\omega = 2^1$. We now give a rigorous general proof of the first conjecture after first establishing the following necessary preliminary results.

Theorem 3. $(u'(\cdot), v')$ solves (13), only if

$$\left[\sum_{x \in X} (u'_i(x))^\omega \right] v'_i = \sum_{x \in X} (u'_i(x))^\omega x. \quad (14)$$

Proof. By a straightforward generalization of the proofs for $\omega = 1$ and 2 given in [1]. Details are omitted in the interest of brevity.

*Theorem 4.*² If $(u'(\cdot), v')$ solves (13), then

$$J_\omega(u'(\cdot), v') = \frac{1}{2} \sum_{i=1}^k \frac{1}{\sum_{x \in X} (u'_i(x))^\omega} \sum_{x \in X} \sum_{y \in X} [u'_i(x)u'_i(y)]^\omega \|x - y\|^2 \quad (15)$$

Proof. We have

$$[u'_i(x)u'_i(y)]^\omega \|x - y\|^2 = [u'_i(x)u'_i(y)]^\omega [\langle x|x - y \rangle + \langle y|y - x \rangle]$$

therefore, with reference to (14)

$$\begin{aligned} \sum_{x \in X} \sum_{y \in X} [u'_i(x)u'_i(y)]^\omega \|x - y\|^2 &= 2 \sum_{x \in X} [u'_i(x)]^\omega \sum_{x \in X} [u'_i(x)]^\omega \langle x|x - v'_i \rangle \\ &= 2 \sum_{x \in X} [u'_i(x)]^\omega \sum_{x \in X} [u'_i(x)]^\omega \|x - v'_i\|^2. \end{aligned} \quad (16)$$

Equation (15) now follows at once from (16) and (12).

Theorem 5. Let $P = \{X_1, \dots, X_k\}$ denote an arbitrary k -partition of X , let $u'(\cdot)$ denote an optimal fuzzy partition for J_ω , and let n = number of elements in X . Then,

$$\frac{2n}{[\alpha(k, P)]^2} \geq \sum_{i=1}^k \min_{1 \leq q \leq k} \left\{ \sum_{x \in X - X_q} (u'_i(x))^\omega \right\}. \quad (17)$$

Proof. Let $u_i(\cdot)$ denote the characteristic function of $X_i \in P$, let $u(\cdot) = \{u_1(\cdot), \dots, u_k(\cdot)\}$, let $v_i = \bar{x}_i$ = centroid of X_i , and let $v = \{v_1, \dots, v_k\}$. Then $u(\cdot) \in \phi(k) \subset \phi_f(k)$, $v \in \mathcal{L}^k$, and we therefore have:

¹When $\omega = 1$, the optimal fuzzy partition typically consists of characteristic functions (i.e., $u'(\cdot) \in \phi(k) \subset \phi_f(k)$) for all values of $\bar{\alpha}$; in other words, the solutions of the relaxed minimization problem (13) typically coincide with the solutions of the original minimization problem (10), regardless of whether $\bar{\alpha}$ is large or small. For this reason, the extension (12) corresponding to $\omega = 1$ is not useful from the standpoint of detecting the presence or absence of separated clusters in X . This point is discussed at length in [1].

²An analogous result holds for the standard k -means criterion in (10); cf. [3].

$$\begin{aligned}
J_{\omega}(u'(\cdot), v') &\leq J_{\omega}(u(\cdot), v) \\
&= \sum_{i=1}^k \sum_{x \in X} [u_i(x)]^{\omega} \|x - v_i\|^2 \\
&= \sum_{i=1}^k \sum_{X_i} \|x - \bar{x}_i\|^2.
\end{aligned}$$

Since $\bar{x}_i \in \text{Co}X_i$, it follows that

$$\|x - \bar{x}_i\|^2 \leq [\text{diam}(X_i)]^2$$

(see eq. (7) in the proof of Theorem 2). Consequently, if n_i = number of elements in X_i , we have,

$$J_{\omega}(u'(\cdot), v') \leq \sum_{i=1}^k n_i [\text{diam}(X_i)]^2$$

and therefore

$$\begin{aligned}
J_{\omega}(u'(\cdot), v') &\leq n \max_{1 \leq p \leq k} [\text{diam}(X_p)]^2 \\
&= n \left[\max_{1 \leq p \leq k} \text{diam}(X_p) \right]^2.
\end{aligned} \tag{18}$$

On the other hand, by Theorem 4, we have

$$\begin{aligned}
J_{\omega}(u'(\cdot), v') &= \frac{1}{2} \sum_{i=1}^k \frac{1}{\sum_{x \in X} (u'_i(x))^{\omega}} \sum_{q=1}^k \sum_{r=1}^k \sum_{x \in X_q} \sum_{y \in X_r} [u'_i(x) u'_i(y)]^{\omega} \|x - y\|^2 \\
&\geq \frac{1}{2} \sum_{i=1}^k \frac{1}{\sum_{x \in X} (u'_i(x))^{\omega}} \sum_{q=1}^k \sum_{\substack{r=1 \\ r \neq q}}^k \sum_{x \in X_q} \sum_{y \in X_r} [u'_i(x) u'_i(y)]^{\omega} [\text{dist}(X_q, X_r)]^2 \\
&\geq \frac{1}{2} \left\{ \sum_{i=1}^k \min_{1 \leq q \leq k} \sum_{x \in X - X_q} (u'_i(x))^{\omega} \right\} \cdot \min_{1 \leq q \leq k} \min_{\substack{1 \leq r \leq k \\ r \neq q}} [\text{dist}(X_q, X_r)]^2.
\end{aligned} \tag{19}$$

The inequality (17) now follows at once from (18), (19), and (2).

(Q.E.D.)

Corollary. If $P' = \{X'_1, \dots, X'_k\}$ is a maximally separated partition relative to α , then for $1 \leq i \leq k$

$$0 \leq \min_{1 \leq q \leq k} \sum_{x \in X_q} (u'_i(x))^\omega \leq \frac{2n}{[\bar{\alpha}(k)]^2}. \quad (20)$$

As an immediate consequence of (20), we have for $1 \leq i \leq k$,

$$x \notin X'_{\gamma(i)} \Rightarrow 0 \leq u'_i(x) \leq \left(\frac{2n}{[\bar{\alpha}(k)]^2} \right)^{1/\omega}. \quad (21)$$

where $\gamma(i)$ satisfies

$$\sum_{x \in X'_{\gamma(i)}} (u'_i(x))^\omega = \min_{1 \leq q \leq k} \sum_{x \in X'_q} (u'_i(x))^\omega \quad (22)$$

Although the upper bound in (21) is coarse, it clearly shows that $u_i(\cdot)$ can be made arbitrarily small on $X - X'_{\gamma(i)}$, by taking $[\bar{\alpha}(k)]$ to be sufficiently large; it also suggests $u_i(\cdot)$ tends to toward 1 on $X'_{\gamma(i)}$ with increasing $\bar{\alpha}$, provided γ is a one-to-one mapping of $\{1, \dots, k\}$ onto itself. In order to establish this last condition, we require the following simple.

Lemma 1. Let $P = \{X_1, \dots, X_k\}$ be any family of subsets of X and let γ be any mapping of $\{1, \dots, k\}$ into itself. Then

$$\bigcap_{i=1}^k (X - X_{\gamma(i)}) = X - \bigcup_{i=1}^k X_{\gamma(i)}. \quad (23)$$

Proof. $X - X_{\gamma(i)} \triangleq \bar{X}_{\gamma(i)}$ = complement of $X_{\gamma(i)}$ in X . Therefore

$$\begin{aligned} \bigcap_{i=1}^k (X - X_{\gamma(i)}) &= \bigcap_{i=1}^k \bar{X}_{\gamma(i)} \\ &= \overline{\left(\bigcup_{i=1}^k X_{\gamma(i)} \right)} \\ &= X - \bigcup_{i=1}^k X_{\gamma(i)}. \end{aligned} \quad (\text{Q.E.D.})$$

Theorem 6. Let ϵ denote an arbitrary positive number smaller than 1, i.e.,

$$0 < \epsilon < 1$$

and let $\bar{\alpha}$ be so large that for $1 \leq i \leq k$

$$x \notin X'_{\gamma(i)} \Rightarrow 0 \leq u'_i(x) \leq \frac{\epsilon}{k} \quad (24)$$

where $X'_{\gamma(i)} \in P'$ = maximally separated k -partition relative to α [see (21)] and where γ satisfies condition (22). Then γ is one-to-one, and for $1 \leq i \leq k$,

$$x \in X'_{\gamma(i)} \Rightarrow 1 - \frac{(k-1)}{k} \epsilon \leq u'_i(x) \leq 1. \quad (25)$$

Proof. Suppose γ is not one-to-one; then $\bigcup_{i=1}^k X'_{\gamma(i)}$ does not exhaust X . Therefore by Lemma 1,

$$\bigcap_{i=1}^k (X - X'_{\gamma(i)}) \neq \phi(\text{empty set}).$$

It follows from (24) that for some $x^* \in \bigcap_{i=1}^k (X - X'_{\gamma(i)})$,

$$\sum_{i=1}^k u'_i(x^*) < \sum_{i=1}^k \frac{\epsilon}{k} < \epsilon < 1$$

which contradicts condition (11)iii. Thus γ is one-to-one and we therefore have for $1 \leq i \leq k$,

$$\bigcap_{\substack{\ell=1 \\ \ell \neq i}}^k (X - X'_{\gamma(\ell)}) = X - \bigcup_{\substack{\ell=1 \\ \ell \neq i}}^k X'_{\gamma(\ell)} = X'_{\gamma(i)}.$$

In view of (24) and (11)iii, it follows that for $1 \leq i \leq k$,

$$\begin{aligned} x \in X'_{\gamma(i)} &\Rightarrow 1 \geq u'_i(x) = 1 - \sum_{\substack{\ell=1 \\ \ell \neq i}}^k u'_\ell(x) \\ &\geq 1 - \left(\frac{k-1}{k}\right)\epsilon. \end{aligned} \quad (\text{Q.E.D.})$$

Theorem 6 shows that the membership functions $u'_i(\cdot)$ in an optimal fuzzy partition for (13) will approximate the characteristic functions of some permutation of the subsets X'_i in a maximally separated k -partition P' , with arbitrarily high accuracy as $\bar{\alpha}(k)$ increases without bound.

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Received September, 1973