Evidential Clustering: a Review of Some New Developments

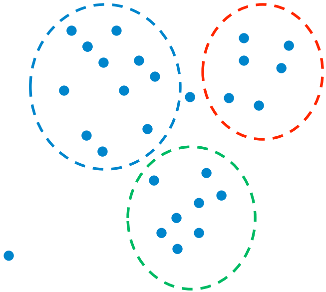
Thierry Denœux

Université de Technologie de Compiègne
HEUDIASYC (UMR CNRS 6599)

https://www.hds.utc.fr/~tdenoeux

4th International Conference on Belief Functions
Prague, CZ
September 21, 2016

Clustering



- n objects described by
  - Attribute vectors $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$ (attribute data) or
  - Dissimilarities (proximity data)
- Goals:
  1. Discover groups in the data
  2. Assess the uncertainty in group membership

Hard and soft clustering concepts

Hard clustering: no representation of uncertainty. Each object is assigned to one and only one group. Group membership is represented by binary variables u_{ik} such that $u_{ik} = 1$ if object i belongs to group k and $u_{ik} = 0$ otherwise.

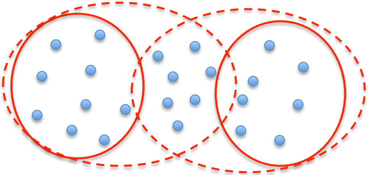
Fuzzy clustering: each object has a degree of membership $u_{ik} \in [0, 1]$ to each group, with $\sum_{k=1}^{c} u_{ik} = 1$. The u_{ik}'s can be interpreted as probabilities.

Fuzzy clustering with noise cluster: the above equality is replaced by $\sum_{k=1}^{c} u_{ik} \leq 1$. The number $1 - \sum_{k=1}^{c} u_{ik}$ is interpreted as a degree of membership (or probability of belonging to) to a noise cluster.

Hard and soft clustering concepts

Possibilistic clustering: the u_{ik} are free to take any value in $[0,1]^c$. Each number u_{ik} is interpreted as a degree of possibility that object i belongs to group k.

Rough clustering: each cluster ω_k is characterized by a lower approximation $\underline{\omega}_k$ and an upper approximation $\overline{\omega}_k$, with $\underline{\omega}_k \subseteq \overline{\omega}_k$; the membership of object i to cluster k is described by a pair $(\underline{u}_{ik}, \overline{u}_{ik}) \in \{0,1\}^2$, with $\underline{u}_{ik} \leq \overline{u}_{ik}$, $\sum_{k=1}^{c} \underline{u}_{ik} \leq 1$ and $\sum_{k=1}^{c} \overline{u}_{ik} \geq 1$.



Clustering and belief functions

clustering structure	uncertainty framework
fuzzy partition	probability theory
possibilistic partition	possibility theory
rough partition	(rough) sets
?	belief functions

- As belief functions extend probabilities, possibilities and sets, could the theory of belief functions provide a more general and flexible framework for cluster analysis?
- Objectives:
  - Unify the various approaches to clustering
  - Achieve a richer and more accurate representation of uncertainty
  - New clustering algorithms and new tools to compare and combine clustering results.

Outline

1. Evidential clustering
   - Credal partition
   - Summarization of a credal partition
   - Relational representation of a credal partition
2. Evidential clustering algorithms
   - Evidential c-means
   - EVCLUS
   - Ek-NNclus
3. Comparing and combining the results of soft clustering algorithms
   - The credal Rand index
   - Combining clustering structures

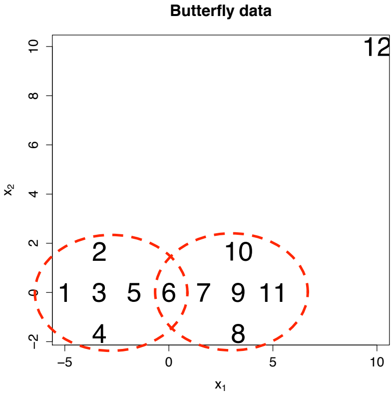
Outline

Outline

Evidential clustering

- Let $O = \{o_1, \ldots, o_n\}$ be a set of n objects and $\Omega = \{\omega_1, \ldots, \omega_c\}$ be a set of c groups (clusters).
- Each object o_i belongs to at most one group.
- Evidence about the group membership of object o_i is represented by a mass function m_i on Ω:
  - for any nonempty set of clusters $A \subseteq \Omega$, $m_i(A)$ is the probability of knowing only that o_i belong to one of the clusters in A.
  - $m_i(\emptyset)$ is the probability of knowing that o_i does not belong to any of the c groups.
- The n-tuple $M = (m_1, \ldots, m_n)$ is called a credal partition.

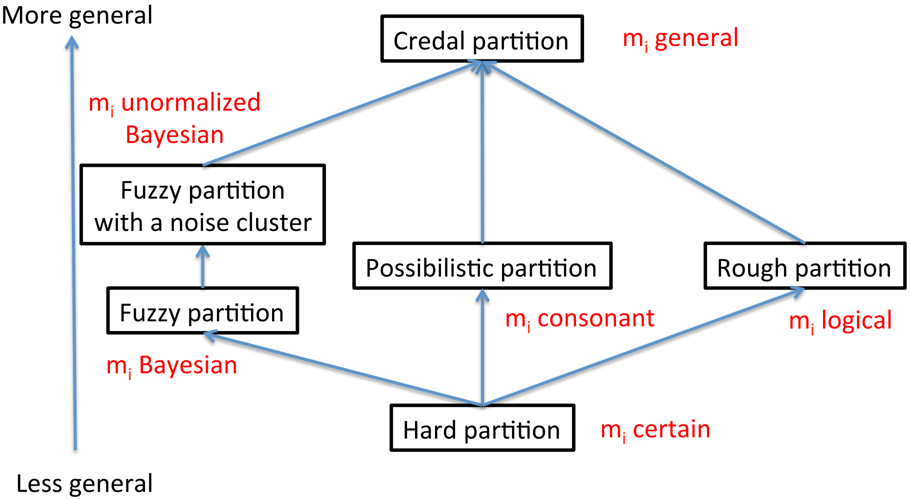
Example



Credal partition

	$\emptyset$	$\{\omega_1\}$	$\{\omega_2\}$	$\{\omega_1, \omega_2\}$
m_3	0	1	0	0
m_5	0	0.5	0	0.5
m_6	0	0	0	1
m_{12}	0.9	0	0.1	0

Relationship with other clustering structures

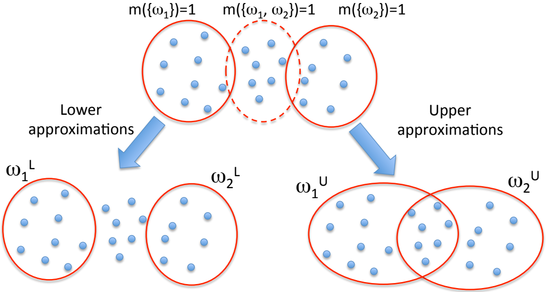


Rough clustering as a special case

- Assume that each m_i is logical, i.e., $m_i(A_i) = 1$ for some $A_i \subseteq \Omega$, $A_i \neq \emptyset$.
- We can then define the lower and upper approximations of cluster ω_k as

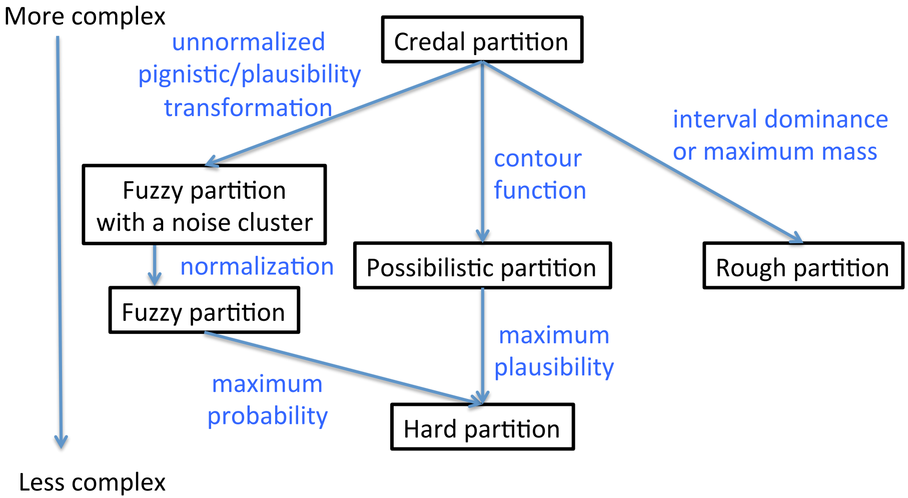
$$\underline{\omega}_k = \{o_i \in O | A_i = \{\omega_k\}\}, \quad \overline{\omega}_k = \{o_i \in O | \omega_k \in A_i\}.$$

- The membership values to the lower and upper approximations of cluster ω_k are $\underline{u}_{ik} = Bel_i(\{\omega_k\})$ and $\overline{u}_{ik} = Pl_i(\{\omega_k\})$.



Outline

Summarization of a credal partition



From evidential to rough clustering

- For each i, let $A_i \subseteq \Omega$ be the set of non dominated clusters

$$A_i = \{\omega \in \Omega | \forall \omega' \in \Omega, Bel_i^*(\{\omega'\}) \leq Pl_i^*(\{\omega\})\},$$

where Bel_i^* and Pl_i^* are the normalized belief and plausibility functions.

- Lower approximation:

$$\underline{u}_{ik} = \begin{cases} 1 & \text{if } A_i = \{\omega_k\} \\ 0 & \text{otherwise.} \end{cases}$$

- Upper approximation:

$$\overline{u}_{ik} = \begin{cases} 1 & \text{if } \omega_k \in A_i \\ 0 & \text{otherwise.} \end{cases}$$

- The outliers can be identified separately as the objects for which $m_i(\emptyset) \geq m_i(A)$ for all $A \neq \emptyset$.

Outline

Relational representation of a hard partition

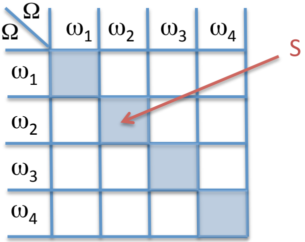
- A hard partition can be represented equivalently by
  - the $n \times c$ membership matrix $U = (u_{ik})$ or
  - an $n \times n$ relation matrix $R = (r_{ij})$ representing the equivalence relation

$$r_{ij} = \begin{cases} 1 & \text{if } o_i \text{ and } o_j \text{ belong to the same group} \\ 0 & \text{otherwise.} \end{cases}$$

- The relational representation R is invariant under renumbering of the clusters, and is thus more suitable to compare or combine several partitions.
- What is the counterpart of matrix R in the case of a credal partition?

Pairwise representation

- Let $M = (m_1, \ldots, m_n)$ be a credal partition.
- For a pair of objects $\{o_i, o_j\}$, let Q_{ij} be the question "Do o_i and o_j belong to the same group?" defined on the frame $\Theta = \{S, \neg S\}$.
- Θ is a coarsening of Ω^2.



Given m_i and m_j on Ω, a mass function m_{ij} on Θ can be computed as follows:

1. Extend m_i and m_j to Ω^2;
2. Combine the extensions of m_i and m_j by the unnormalized Dempster's rule;
3. Compute the restriction of the combined mass function to Θ.

Pairwise mass function

- Mass function:

$$
\begin{aligned}
m_{ij}(\emptyset) &= m_i(\emptyset) + m_j(\emptyset) - m_i(\emptyset)m_j(\emptyset) \\
m_{ij}(\{S\}) &= \sum_{k=1}^{c} m_i(\{\omega_k\})m_j(\{\omega_k\}) \\
m_{ij}(\{\neg S\}) &= \kappa_{ij} - m_{ij}(\emptyset) \\
m_{ij}(\Theta) &= 1 - \kappa_{ij} - \sum_{k} m_i(\{\omega_k\})m_j(\{\omega_k\}).
\end{aligned}
$$

  where κ_{ij} is the degree of conflict between m_i and m_j.

- In particular,

$$pl_{ij}(S) = 1 - \kappa_{ij}.$$

Return to CECM

Special cases

Hard partition:

$$m_{ij}(\{S\}) = r_{ij}, \quad m_{ij}(\{\neg S\}) = 1 - r_{ij} \quad \text{with } r_{ij} \in \{0, 1\}$$

Fuzzy partition:

$$m_{ij}(\{S\}) = r_{ij}, \quad m_{ij}(\{\neg S\}) = 1 - r_{ij} \quad \text{with } r_{ij} \in [0, 1]$$

Rough partition: Assume $m_i(A_i) = 1$ and $m_j(A_j) = 1$.

$$\begin{aligned} m_{ij}(\{S\}) &= 1 \quad \text{if } A_i = A_j = \{\omega_k\} \\ m_{ij}(\{\neg S\}) &= 1 \quad \text{if } A_i \cap A_j = \emptyset \\ m_{ij}(\Theta) &= 1 \quad \text{otherwise.} \end{aligned}$$

Pairwise representation of a credal partition

- Let $M = (m_1, \ldots, m_n)$ be a credal partition.
- The tuple $R = (m_{ij})_{1 \leq i < j \leq n}$ is called the pairwise representation of credal partition M.

$$M = (m_1, m_2, m_3, m_4, m_5) \longrightarrow R = \begin{pmatrix} & 1 & 2 & 3 & 4 & 5 \\ 1 & \cdot & m_{12} & m_{13} & m_{14} & m_{15} \\ 2 & \cdot & \cdot & m_{23} & m_{24} & m_{25} \\ 3 & \cdot & \cdot & \cdot & m_{34} & m_{35} \\ 4 & \cdot & \cdot & \cdot & \cdot & m_{45} \\ 5 & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

- Open question: given a pairwise representation R, can we uniquely recover the credal partition M, up to a permutation of the cluster indices?

Outline

Main approaches

1. Evidential *c*-means (ECM): (Masson and Denoeux, 2008):
   - Attribute data
   - HCM, FCM family
2. EVCLUS (Denoeux and Masson, 2004; Denoeux et al., 2016):
   - Attribute or proximity (possibly non metric) data
   - Multidimensional scaling approach
3. EK-NNclus (Denoeux et al, 2015)
   - Attribute or proximity data
   - Searches for the most plausible partition of a dataset

Outline

Principle

- Problem: generate a credal partition $M = (m_1, \ldots, m_n)$ from attribute data $X = (\boldsymbol{x}_1, ..., \boldsymbol{x}_n)$, $\boldsymbol{x}_i \in \mathbb{R}^p$.
- Generalization of hard and fuzzy c-means algorithms:
  - Each cluster is represented by a prototype.
  - Cyclic coordinate descent algorithm: optimization of a cost function alternatively with respect to the prototypes and to the credal partition.

Fuzzy c-means (FCM)

- Minimize

$$J_{\text{FCM}}(U,V)=\sum_{i=1}^{n}\sum_{k=1}^{c}u_{ik}^{\beta}d_{ik}^{2}$$

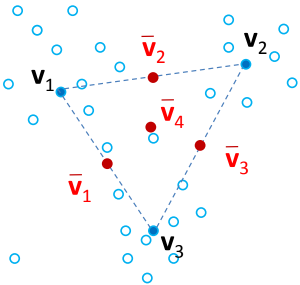
  with $d_{ik}=||\boldsymbol{x}_i-\boldsymbol{v}_k||$ subject to the constraints $\sum_k u_{ik}=1$ for all i.
- Alternate optimization algorithm:

$$\boldsymbol{v}_k=\frac{\sum_{i=1}^{n}u_{ik}^{\beta}\boldsymbol{x}_i}{\sum_{i=1}^{n}u_{ik}^{\beta}}$$

$$u_{ik}=\frac{d_{ik}^{-2/(\beta-1)}}{\sum_{\ell=1}^{c}d_{i\ell}^{-2/(\beta-1)}}.$$

ECM algorithm

Principle



- Each cluster ω_k represented by a prototype $\boldsymbol{v}_k$.
- Each nonempty set of clusters A_j represented by a prototype $\bar{\boldsymbol{v}}_j$ defined as the center of mass of the $\boldsymbol{v}_k$ for all $\omega_k \in A_j$.
- Basic ideas:
  - For each nonempty $A_j \in \Omega$, $m_{ij} = m_i(A_j)$ should be high if $\boldsymbol{x}_i$ is close to $\bar{\boldsymbol{v}}_j$.
  - The distance to the empty set is defined as a fixed value δ.

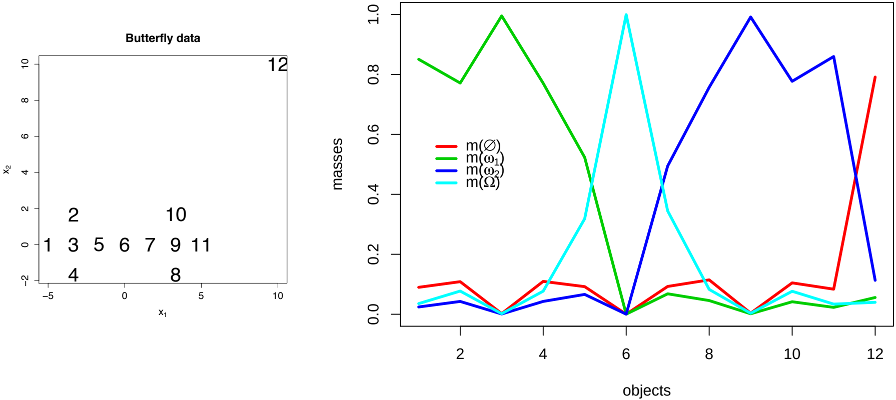
ECM algorithm: objective criterion

- Define the nonempty focal sets $\mathcal{F} = \{A_1, \ldots, A_f\} \subseteq 2^\Omega \setminus \{\emptyset\}$.
- Minimize

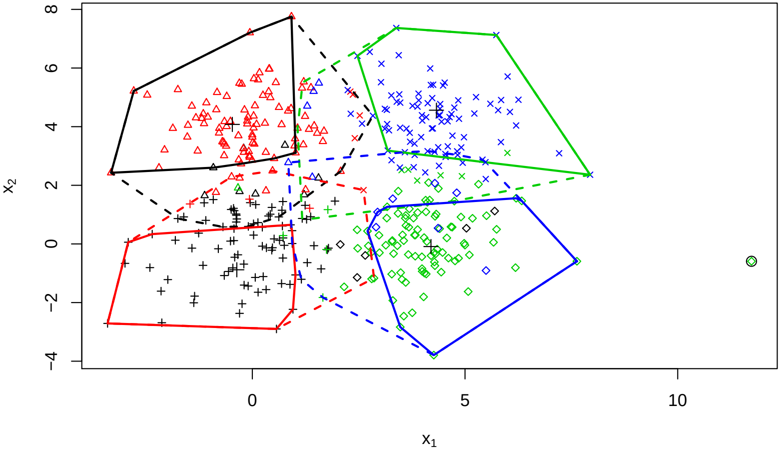
$$J_{\text{ECM}}(M, V) = \sum_{i=1}^{n} \sum_{j=1}^{f} |A_j|^\alpha m_{ij}^\beta d_{ij}^2 + \sum_{i=1}^{n} \delta^2 m_{i\emptyset}^\beta$$

  subject to the constraints $\sum_{j=1}^{f} m_{ij} + m_{i\emptyset} = 1$ for all i.
- Parameters:
  - α controls the specificity of mass functions (default: 1)
  - β controls the hardness of the credal partition (default: 2)
  - δ controls the proportion of data considered as outliers
- $J_{\text{ECM}}(M, V)$ can be iteratively minimized with respect to M and to V.

Butterfly dataset



4-class data set



Determining the number of groups

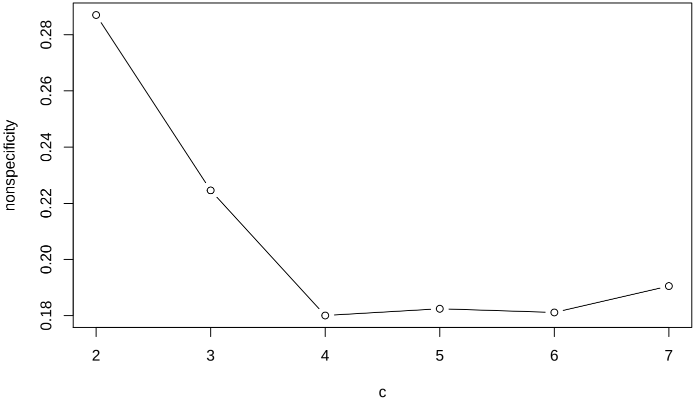
- If a proper number of groups is chosen, the prototypes will cover the clusters and most of the mass will be allocated to singletons of Ω.
- On the contrary, if c is too small or too high, the mass will be distributed to subsets with higher cardinality or to $\emptyset$.
- Nonspecificity of a mass function:

$$N(m) \triangleq \sum_{A \in 2^\Omega \setminus \emptyset} m(A) \log_2 |A| + m(\emptyset) \log_2 |\Omega|$$

- Proposed validity index of a credal partition:

$$N^*(c) \triangleq \frac{1}{n \log_2(c)} \sum_{i=1}^{n} \left[\sum_{A \in 2^\Omega \setminus \emptyset} m_i(A) \log_2 |A| + m_i(\emptyset) \log_2(c) \right]$$

Results for the 4-class dataset



Constrained Evidential *c*-means

- In some cases, we may have some prior knowledge about the group membership of some objects.
- Such knowledge may take the form of instance-level constraints of two kinds:
  1. Must-link (ML) constraints, which specify that two objects certainly belong to the same cluster;
  2. Cannot-link (CL) constraints, which specify that two objects certainly belong to different clusters.
- How to take into account such constraints?

Modified cost-function

- To take into account ML and CL constraints, we can modify the cost function of ECM as

$$J_{\text{CECM}}(M,V) = (1-\xi)J_{\text{ECM}}(M,V) + \xi J_{\text{CONST}}(M)$$

with

$$J_{\text{CONST}}(M) = \frac{1}{|\mathcal{M}|+|\mathcal{C}|}\left[\sum_{(\mathbf{x}_i,\mathbf{x}_j)\in\mathcal{M}} pl_{ij}(\neg S) + \sum_{(\mathbf{x}_i,\mathbf{x}_j)\in\mathcal{C}} pl_{ij}(S)\right]$$

where
  - $\mathcal{M}$ and $\mathcal{C}$ are, respectively, the sets of ML and CL constraints.
  - $pl_{ij}(S)$ and $pl_{ij}(\neg S)$ are computed from the pairwise mass function m_{ij}

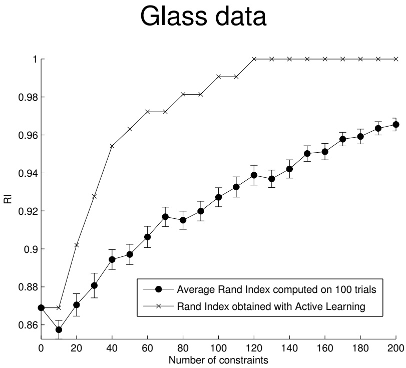
Go back to pairwise mass functions

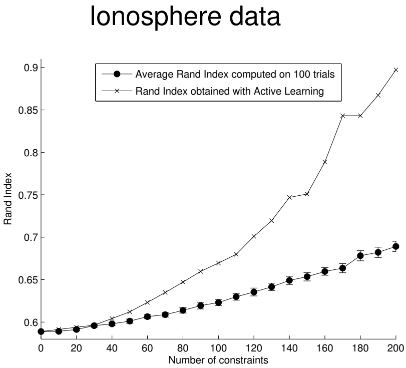
- Minimizing $J_{\text{CECM}}(M,V)$ w.r.t. M is a quadratic programming problem.

Active learning

- ML and CL constraints are sometimes given in advance, but they can sometimes be elicited from the user using an active learning strategy.
- For instance, we may select pairs of object such that
  - The first object is classified with high uncertainty (e.g., an object such that m_i has high nonspecificity);
  - The second object is classified with low uncertainty (e.g., an object that is close to a cluster center).
- The user is then provided with this pair of objects, and enters either a ML or a CL constraint.

Results


Glass data
RI
Number of constraints
1
0.98
0.96
0.94
0.92
0.9
0.88
0.86
0
20
40
60
80
100
120
140
160
180
200
Average Rand Index computed on 100 trials
Rand Index obtained with Active Learning


Ionosphere data
Rand Index
Number of constraints
0.9
0.85
0.8
0.75
0.7
0.65
0.6
0
20
40
60
80
100
120
140
160
180
200
Average Rand Index computed on 100 trials
Rand Index obtained with Active Learning

Other variants of ECM

Relational Evidential c-Means (RECM) for (metric) proximity data (Masson and Denœux, 2009).

ECM with adaptive metrics to obtain non-spherical clusters (Antoine et al., 2012). Specially useful with CECM.

Spatial Evidential C-Means (SECM) for image segmentation (Lelandais et al., 2014).

Credal c-means (CCM) : different definition of the distance between a vector and a meta-cluster (Liu et al., 2014).

Median evidential c-means (MECM) : different cost criterion, extension of the median hard and fuzzy c-means (Zhou et al., 2015).

Outline

Learning a Credal Partition from proximity data

- Problem: given the dissimilarity matrix $D = (d_{ij})$, how to build a "reasonable" credal partition ?
- We need a model that relates cluster membership to dissimilarities.
- Basic idea: "The more similar two objects, the more plausible it is that they belong to the same group".
- How to formalize this idea?

Formalization

- Let m_i and m_j be mass functions regarding the group membership of objects o_i and o_j.
- We have seen that the plausibility that objects o_i and o_j belong to the same group is

$$pl_{ij}(S) = \sum_{A \cap B \neq \emptyset} m_i(A) m_j(B) = 1 - \kappa_{ij}$$

  where κ_{ij} = degree of conflict between m_i and m_j.
- Problem: find a credal partition $M = (m_1, \ldots, m_n)$ such that larger degrees of conflict κ_{ij} correspond to larger dissimilarities d_{ij}.

Cost function

- Approach: minimize the discrepancy between the dissimilarities d_{ij} and the degrees of conflict κ_{ij}.
- Example of a cost (stress) function:

$$J(M) = \sum_{i<j} (\kappa_{ij} - \varphi(d_{ij}))^2$$

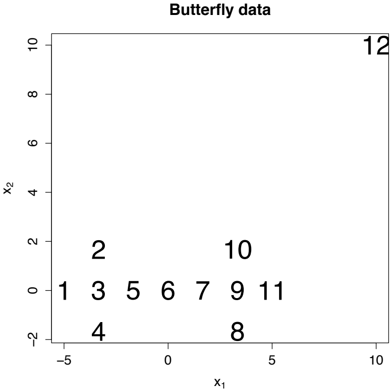
where φ is an increasing function from $[0, +\infty)$ to $[0, 1]$, for instance

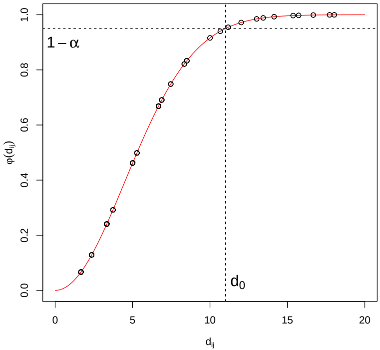
$$\varphi(d) = 1 - \exp(-\gamma d^2).$$

Butterfly example

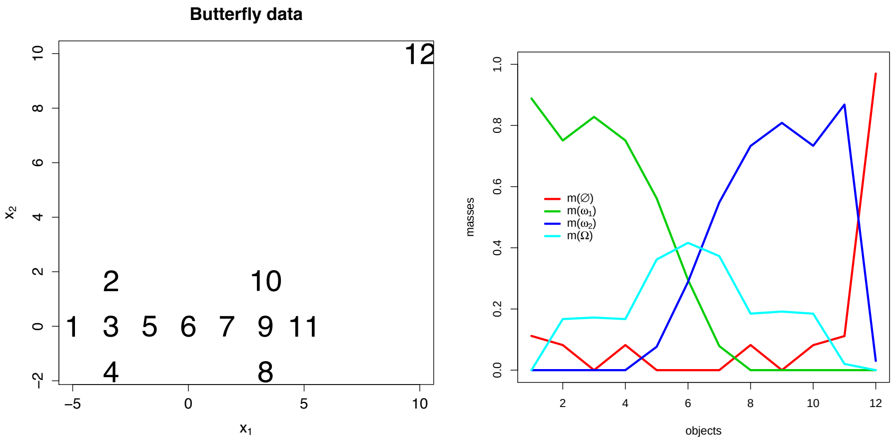
Data and dissimilarities

Determination of γ in $\varphi(d) = 1 - \exp(-\gamma d^2)$: fix $\alpha \in (0,1)$ and d_0 such that, for any two objects (o_i, o_j) with $d_{ij} \geq d_0$, the plausibility that they belong to the same cluster is at least $1 - \alpha$.



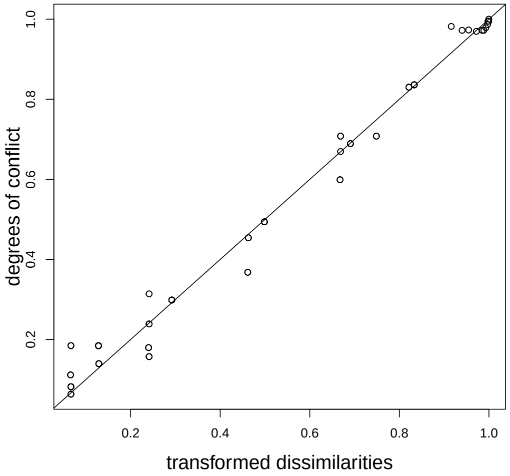


Butterfly example
Credal partition

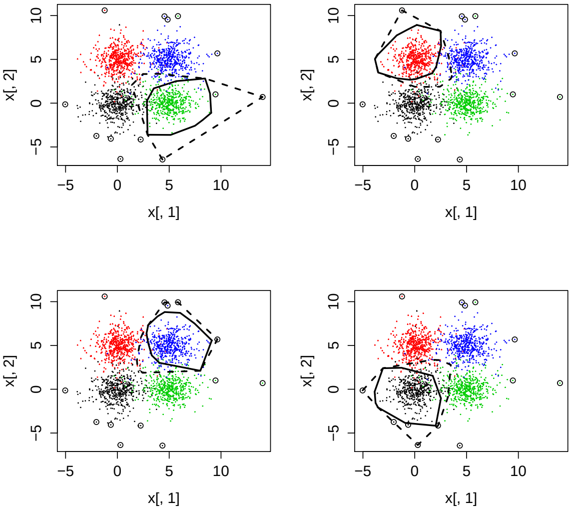


Butterfly example

Shepard diagram



Example with a four-class dataset (2000 objects)



Modifications of EVCLUS for large datasets

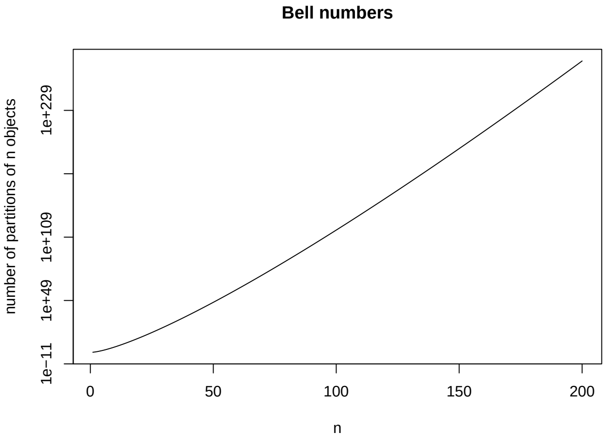
- Initially, EVCLUS used a gradient descent algorithm to minimize the stress function, and it required to store the whole dissimilarity matrix: it was limited to small sets of proximity data (a few hundreds of objects).
- Recent improvements to EVCLUS make it applicable to large datasets ($\sim 10^4 - 10^5$ objects and hundreds of classes).
- More on this in tomorrow's presentation.

Outline

Reasoning in the space of all partitions

- Assuming there is a true unknown partition, our frame of discernment should be the set $\mathcal{R}$ of all equivalent relations ($\equiv$ partitions) of the set of n objects.
- But this set is huge!

Number of partitions of *n* objects



Can we implement evidential reasoning in such a large space?

Model

- Evidence: $n \times n$ matrix $D = (d_{ij})$ of dissimilarities between the n objects.
- Assumptions
  1. Two objects have all the more chance to belong to the same group, that they are more similar:

$$
\begin{aligned}
m_{ij}(\{S\}) &= \varphi(d_{ij}), \\
m_{ij}(\Theta) &= 1 - \varphi(d_{ij}),
\end{aligned}
$$

     where φ is a non-increasing mapping from $[0, +\infty)$ to $[0, 1)$.
  2. The mass functions m_{ij} are independent.
- How to combine these $n(n-1)/2$ mass functions to find the most plausible partition of the n objects?

Evidence combination

- Let $\mathcal{R}_{ij}$ denote the set of partitions of the n objects such that objects o_i and o_j are in the same group ($r_{ij} = 1$).
- Each mass function m_{ij} can be vacuously extended to the space $\mathcal{R}$ of equivalence relations:

$$\begin{array}{rcl} m_{ij}(\{S\}) & \longrightarrow & \mathcal{R}_{ij} \\ m_{ij}(\Theta) & \longrightarrow & \mathcal{R} \end{array}$$

- The extended mass functions can then be combined by Dempster's rule.
- Resulting contour function:

$$pl(R) \propto \prod_{i<j} (1 - \varphi(d_{ij}))^{1-r_{ij}}$$

for any $R \in \mathcal{R}$.

Decision

- The logarithm of the contour function can be written as

$$\log pl(R) = -\sum_{i<j} r_{ij} \log(1 - \varphi(d_{ij})) + C$$

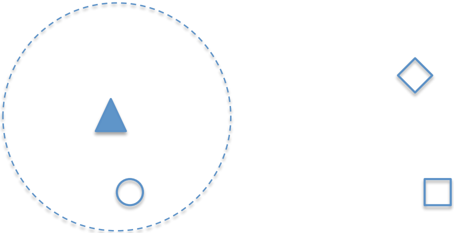
- Finding the most plausible partition is thus a binary linear programming problem. It can be solves exactly only for small n.
- However, the problem can be solved approximately using a heuristic greedy search procedure: the Ek-NNclus algorithm.
- This is a decision-directed clustering procedure, using the evidential k-nearest neighbor (Ek-NN) rule as a base classifier.

Example

Toy dataset

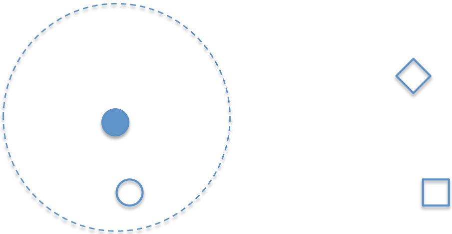
Example

Iteration 1



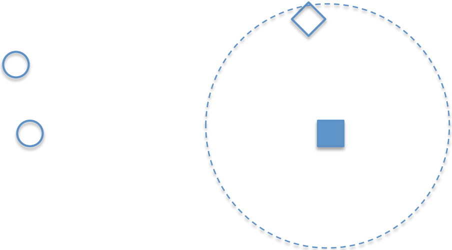
Example

Iteration 1 (continued)



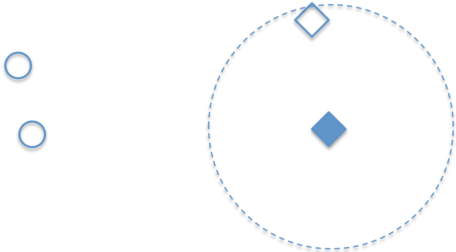
Example

Iteration 2



Example

Iteration 2 (continued)



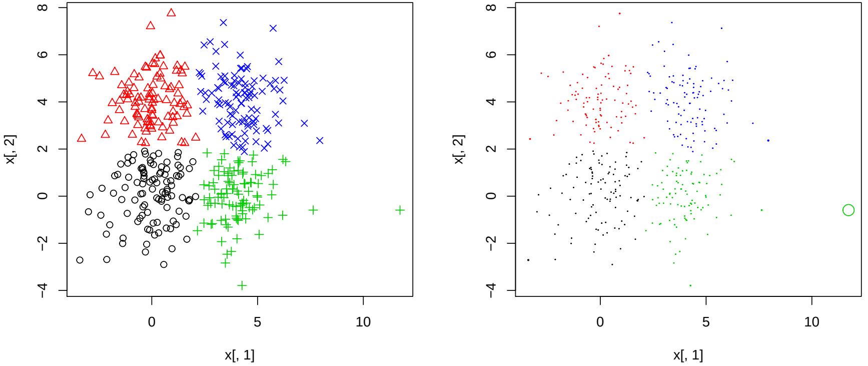
Example

Result

Ek-NNclus

- Starting from a random initial partition, classify each object in turn, using the Ek-NN rule.
- The algorithm converges to a local maximum of the contour function $pl(R)$ if $k = n - 1$.
- With $k < n - 1$, the algorithm converges to a local maximum of an objective function that approximates $pl(R)$.
- Implementation details:
  - Number k of neighbors: two to three times $\sqrt{n}$.
  - $\varphi(d) = 1 - \exp(-\gamma d^2)$, with γ fixed to the inverse of the q-quantile of the distances d_{ij}^2 between an object and its k NN. Typically, $q \geq 0.5$.
  - The number of clusters does not need to be fixed in advance.

Example



Outline

Exploiting the generality of evidential clustering

- We have seen that the concept of credal partition subsumes the main hard and soft clustering structures.
- Consequently, methods designed to evaluate or combine credal partitions can be used to evaluate or combine the results of any hard or soft clustering algorithms.
- Two such methods will be described:
  1. A generalization of the Rand index to compute the distance between two credal partitions;
  2. A method to combine credal partitions.

Outline

1. Evidential clustering
   - Credal partition
   - Summarization of a credal partition
   - Relational representation of a credal partition
2. Evidential clustering algorithms
   - Evidential *c*-means
   - EVCLUS
   - E*k*-NNclus
3. Comparing and combining the results of soft clustering algorithms
   - The credal Rand index
   - Combining clustering structures

Rand index

- The Rand index is a widely used measure of agreement (similarity) tbetween two hard partitions.
- It is defined as

$$RI = \frac{a+b}{n(n-1)/2}$$

  with
  - $a =$ number of pairs of objects that are grouped together in both partitions
  - $b =$ number of pairs of objects that are assigned to different clusters in both partitions.
- How to generalize the Rand Index to credal partitions?

Jousselme's distance

- Let $R = (m_{ij})$ and $R' = (m'_{ij})$ be the pairwise representations of two credal partitions.
- The assess the distance between R and R', we can average the distances between the m_{ij}'s and m'_{ij}'s.
- A suitable measure is the squared Jousselme's metric, defined as

$$
\begin{aligned}
d_{ij}^2 &= \frac{1}{2} \sum_{A,B \in \Theta} (m_{ij}(A) - m'_{ij}(A)) \frac{|A \cap B|}{|A \cup B|} \\
&= \frac{1}{2} \boldsymbol{m}_{ij}^T J \, \boldsymbol{m}'_{ij}
\end{aligned}
$$

with $\boldsymbol{m}_{ij} = (m_{ij}(\emptyset), m_{ij}(\{s\}), m_{ij}(\{ns\}), m_{ij}(\Theta))^T$ and

$$
J = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \\ 0 & 1/2 & 1/2 & 1 \end{pmatrix}
$$

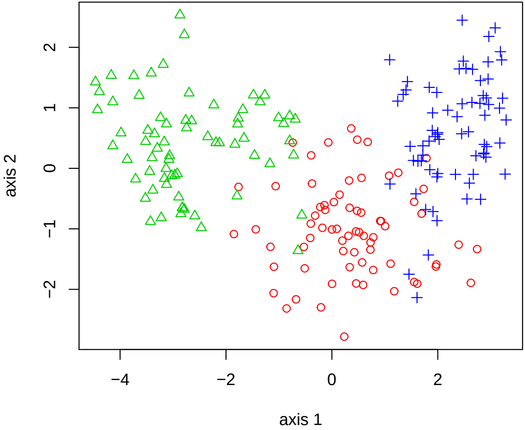
Credal Rand index

- We define the Credal Rand Index as

$$CRI = 1 - \frac{\sum_{i<j} d_{ij}^2}{n(n-1)/2}.$$

- Properties:
  - $0 \leq CRI \leq 1$
  - CRI is the Rand index when the two partitions are hard
  - Symmetry: $CRI(R, R') = CRI(R', R)$
  - If $R = R'$, then $CRI(R, R') = 1$
  - 1-CRI is a squared distance between R and R'
- The CRI can be used to compare the results of any two hard or soft clustering algorithms.

Example: Seeds data



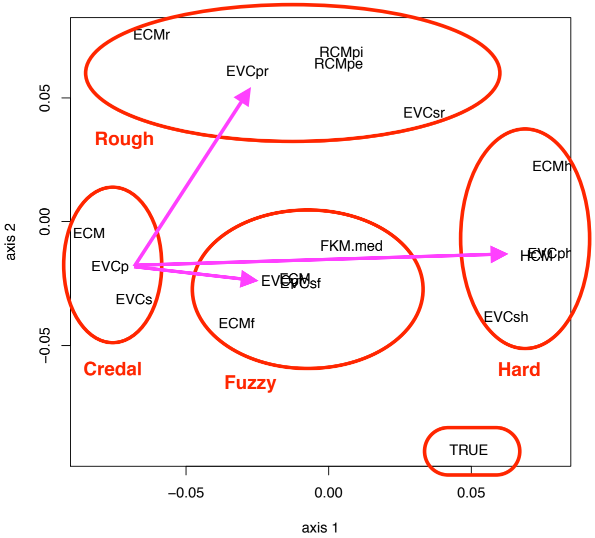
- Seeds from three different varieties of wheat: Kama, Rosa and Canadian, 70 elements each
- 7 features

Clustering algorithms

- Evidential clustering (R package `evclust`)
  - ECM, $\mathcal{F} = \{A \subseteq \Omega, |A| \leq 2\}$
  - EVCLUS ($\mathcal{F} = \{A \subseteq \Omega, |A| \leq 1\} \cup \{\Omega\}$; $\mathcal{F} = 2^{\Omega}$).

  and their derived hard, fuzzy and rough partitions
- Hard clustering: HCM (R package `stats`)
- Fuzzy clustering (R package `fclust`)
  - FCM
  - Fuzzy *K* medoids
- Rough clustering (R package `SoftClustering`)
  - Peter's rough *k*-means P-RCM
  - Pi rough *k*-means π-RCM

Result: MDS configuration

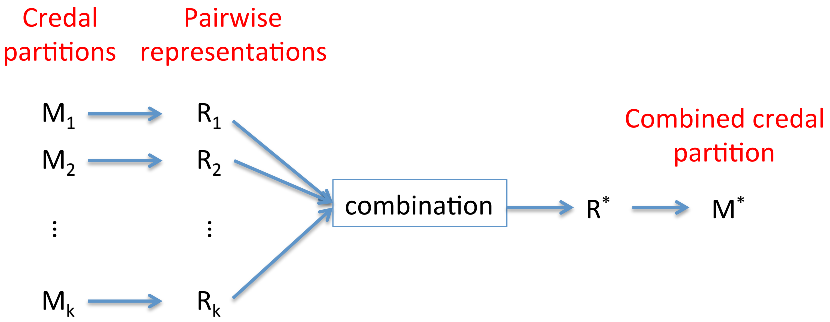


Outline

Motivations for combining clustering structures

- Let $M_1, \ldots, M_N$ be an ensemble of N credal partitions generated by hard or soft (fuzzy, rough, etc.) clustering structures.
- It may be useful to combine these credal partitions:
  - to increase the chance of finding a good approximation to the true partition, or
  - to highlight invariant patterns across the clustering structures.
- Combination is easily carried out using pairwise representations.

Combination method



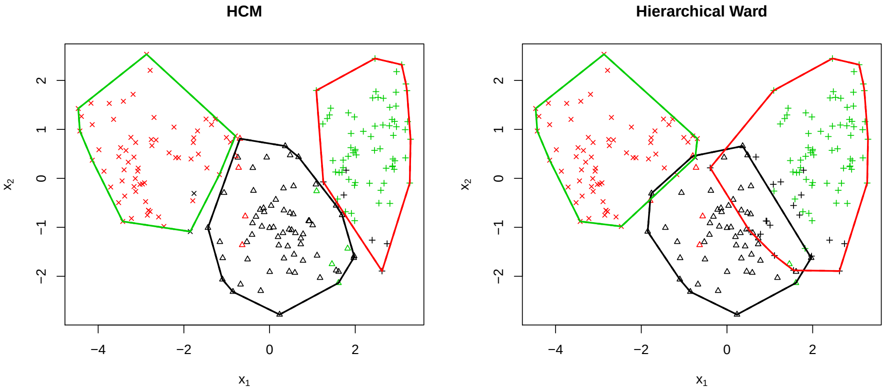
The combined credal partition can be defined as

$$M^* = \arg\max_M CRI(\mathcal{R}(M), R^*),$$

where $\mathcal{R}(M)$ denotes the pairwise representation of M.

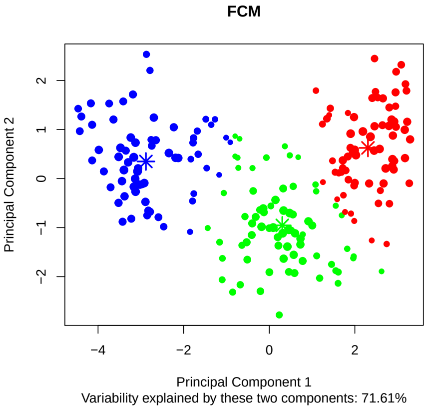
Example: seeds data

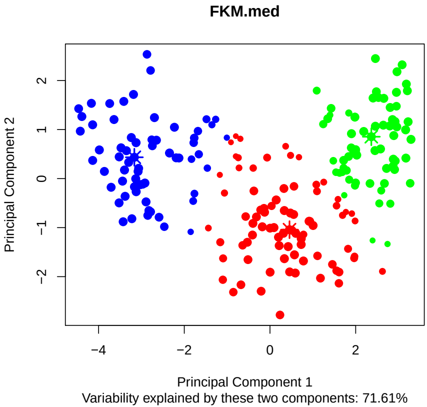
Hard clustering results



Example: seeds data

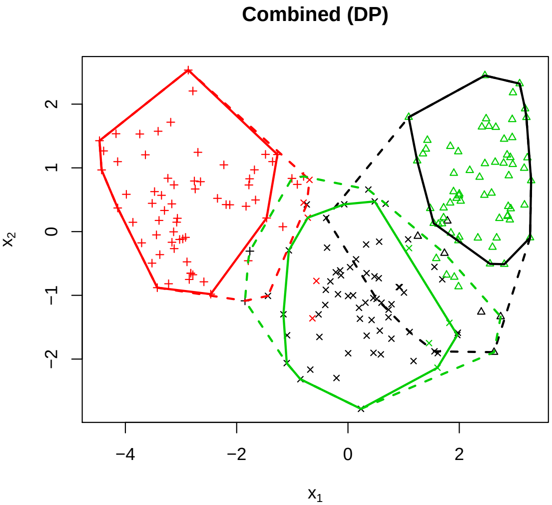
Fuzzy clustering results





Example: seeds data

Combined credal partition (Dubois-Prade rule)



Summary

- The Dempster-Shafer theory of belief functions provides a rich and flexible framework to represent uncertainty in clustering.
- The concept of credal partition encompasses the main existing soft clustering concepts (fuzzy, possibilistic, rough partitions).
- Efficient algorithms exist, allowing one to generate credal partitions from attribute or proximity datasets.
- These algorithms can be applied to large datasets and large numbers of clusters (by carefully selecting the focal sets).
- Concepts from the theory of belief functions make it possible to compare and combine clustering structures generated by various soft clustering algorithms.

Future research directions

- Combining clustering structures in various settings
  - distributed clustering,
  - combination of different attributes, different algorithms,
  - etc.
- Handling huge datasets (several millions of objects)
- Criteria for selecting the number of clusters
- Semi-supervised clustering
- Clustering imprecise or uncertain data
- Applications to image processing, social network analysis, process monitoring, etc.
- Etc...

The `evclust` package

evclust: Evidential Clustering

Various clustering algorithms that produce a credal partition, i.e., a set of Dempster-Shafer mass functions representing the membership of objects to clusters. The mass functions quantify the cluster-membership uncertainty of the objects. The algorithms are: Evidential c-Means (ECM), Relational Evidential c-Means (RECM), Constrained Evidential c-Means (CECM), EVCLUS and EK-NNclus.

Version:	1.0.3
Depends:	R (≥ 3.1.0)
Imports:	FNN, R.utils, limSolve, Matrix
Suggests:	knitr, rmarkdown
Published:	2016-09-04
Author:	Thierry Denoeux
Maintainer:	Thierry Denoeux <tdenoeux at utc.fr>
License:	GPL-3
NeedsCompilation:	no
In views:	Cluster
CRAN checks:	evclust results

`https://cran.r-project.org/web/packages`

References on clustering I

cf. https://www.hds.utc.fr/~tdenoeux

M.-H. Masson and T. Denœux.
ECM: An evidential version of the fuzzy c-means algorithm.
Pattern Recognition, 41(4):1384-1397, 2008.

M.-H. Masson and T. Denœux.
RECM: Relational Evidential c-means algorithm.
Pattern Recognition Letters, 30:1015-1026, 2009.

B. Lelandais, S. Ruan, T. Denoeux, P. Vera, I. Gardin.
Fusion of multi-tracer PET images for Dose Painting.
Medical Image Analysis, 18(7):1247-1259, 2014.

V. Antoine, B. Quost, M.-H. Masson and T. Denoeux.
CECM: Constrained Evidential C-Means algorithm.
Computational Statistics and Data Analysis, 56(4):894-914, 2012.

References on clustering II

cf. https://www.hds.utc.fr/~tdenoeux

- T. Denœux and M.-H. Masson.
  EVCLUS: Evidential Clustering of Proximity Data.
  IEEE Transactions on SMC B, 34(1):95-109, 2004.
- T. Denœux, S. Sriboonchitta and O. Kanjanatarakul
  Evidential clustering of large dissimilarity data.
  Knowledge-Based Systems, 106:179–195, 2016.
- T. Denoeux, O. Kanjanatarakul and S. Sriboonchitta.
  EK-NNclus: a clustering procedure based on the evidential K-nearest neighbor rule.
  Knowledge-Based Systems, Vol. 88, pages 57-69, 2015.