## Classification and clustering using Belief functions

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## Focus of this lecture

- Dempster-Shafer (DS) theory (evidence theory, theory of belief functions):
  - A formal framework for reasoning with partial (uncertain, imprecise) information.
  - Has been applied to statistical inference, expert systems, information fusion, classification, clustering, etc.
- Purpose of these lecture:
  - Brief introduction or reminder on DS theory;
  - Review the application of belief functions to classification and clustering.

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### Dempster-Shafer theory

- Mass, belief and plausibility functions
- Dempster's rule
- Decision analysis

### Evidential classification

- Evidential K-NN rule
- Evidential neural network classifier
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### Evidential clustering

- Evidential partition
- Evidential c-means
- EVCLUS
- Ek-NNclus

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## Dempster-Shafer theory

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## Mass function

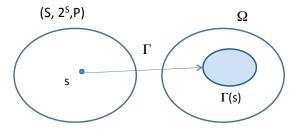
- Let Ω be a finite set called a frame of discernment.
- A mass function is a function  $m: 2^{\Omega} \rightarrow [0, 1]$  such that

$$\sum_{A\subseteq\Omega}m(A)=1.$$

- The subsets A of  $\Omega$  such that  $m(A) \neq 0$  are called the focal sets of m.
- If  $m(\emptyset) = 0$ , *m* is said to be normalized (usually assumed).

## Source

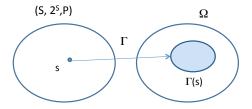
- A mass function is usually induced by a source, defined a 4-tuple (S, 2<sup>S</sup>, P, Γ), where
  - S is a finite set;
  - *P* is a probability measure on  $(S, 2^S)$ ;
  - $\Gamma$  is a multi-valued-mapping from *S* to  $2^{\Omega}$ .



•  $\Gamma$  carries *P* from *S* to  $2^{\Omega}$ : for all  $A \subseteq \Omega$ ,

$$m(A) = P(\{s \in S | \Gamma(s) = A\}).$$

## Interpretation

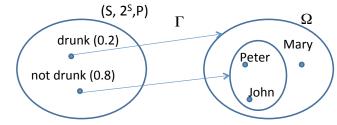


- $\Omega$  is a set of possible states of the world, about which we collect some evidence. Let  $\omega$  be the true state.
- *S* is a set of interpretations of the evidence.
- If s ∈ S holds, we know that ω belongs to the subset Γ(s) of Ω, and nothing more.
- m(A) is then the probability of knowing only that  $\omega \in A$ .
- In particular,  $m(\Omega)$  is the probability of knowing nothing.

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## Example

- A murder has been committed. There are three suspects:  $\Omega = \{Peter, John, Mary\}.$
- A witness saw the murderer going away, but he is short-sighted and he only saw that it was a man. We know that the witness is drunk 20 % of the time.



• We have  $\Gamma(\neg drunk) = \{Peter, John\}$  and  $\Gamma(drunk) = \Omega$ , hence

 $m(\{\text{Peter, John}\}) = 0.8, \quad m(\Omega) = 0.2$ 

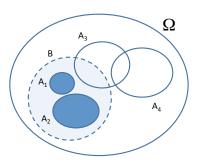
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## Special cases

- A mass function m is said to be:
  - logical if it has only one focal set; it is then equivalent to a set.
  - Bayesian if all focal sets are singletons; it is equivalent to a probability distribution.
- A mass function can thus be seen as
  - a generalized set, or as
  - a generalized probability distribution.

## **Belief function**

 If the evidence tells us that the truth is in A, and A ⊆ B, we say that the evidence supports B.



• Given a normalized mass function *m*, the probability that the evidence supports *B* is thus

$$\textit{Bel}(\textit{B}) = \sum_{\textit{A} \subseteq \textit{B}} \textit{m}(\textit{A})$$

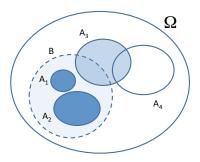
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• The number Bel(B) is called the degree of belief in *B*, and the function  $B \rightarrow Bel(B)$  is called a belief function.

## Plausibility function

• If the evidence does not support  $\overline{B}$ , it is consistent with B.



• The probability that the evidence is consistent with *B* is thus

$$Pl(B) = 1 - Bel(\overline{B})$$
  
 $= \sum_{A \cap B \neq \emptyset} m(A).$ 

• The number PI(B) is called the plausibility of *B*, and the function  $B \rightarrow PI(B)$  is called a plausibility function.

## Two-dimensional representation

- The uncertainty on a proposition *B* is represented by two numbers: Bel(B) and Pl(B), with  $Bel(B) \le Pl(B)$ .
- The intervals [*Bel*(*B*), *Pl*(*B*)] have maximum length when *m* is the vacuous mass function. Then,

[Bel(B), Pl(B)] = [0, 1]

for all subset *B* of  $\Omega$ , except  $\emptyset$  and  $\Omega$ .

 The intervals [Bel(B), Pl(B)] are reduced to points when the focal sets of m are singletons (m is then said to be Bayesian); then,

$$Bel(B) = Pl(B)$$

for all *B*, and *Bel* is a probability measure.

## Consonant mass functions

If the focal sets of *m* are nested (A<sub>1</sub> ⊂ A<sub>2</sub> ⊂ ... ⊂ A<sub>n</sub>), *m* is said to be consonant. *Pl* is then a possibility measure:

$$PI(A \cup B) = \max(PI(A), PI(B))$$

for all  $A, B \subseteq \Omega$  and *Bel* is the dual necessity measure, i.e.,

$$Bel(A \cap B) = min(Bel(A), Bel(B))$$

The corresponding possibility distribution is the contour function

$$pl(\omega) = Pl(\{\omega\})$$
 for all  $\omega \in \Omega$ .

We have

$$PI(A) = \max_{\omega \in A} pI(\omega)$$
 for all  $A \subseteq \Omega$ .

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## Belief-probability transformations

- It may be useful to transform a mass function *m* into a probability distribution for approximation or decision-making.
- Two main belief-probability transformations:
  - Plausibility-probability transformation

$$p_m(\omega) = rac{pl(\omega)}{\sum_{\omega \in \Omega} pl(\omega)}$$

Property:  $p_{m_1 \oplus m_2} = p_{m_1} \oplus p_{m_2}$ . Pignistic transformation

$$betp_m(\omega) = \sum_{A \ni \omega} \frac{m(A)}{|A|}$$

Property: The corresponding probability measure  $Betp_m$  is the center of mass of all probability measures P such that  $Bel \leq P \leq Pl$ .

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## Summary

- A probability measure is precise, in so far as it represents the uncertainty of the proposition  $\omega \in A$  by a single number P(A).
- In contrast, a mass function is imprecise (it assigns probabilities to subsets).
- As a result, in DS theory, the uncertainty about a subset A is represented by two numbers (Bel(A), Pl(A)), with Bel(A) ≤ Pl(A).
- This model has some connections with possibility theory (it is more general) and with rough set theory, in which a set is approximated by lower and upper approximations, due to coarseness of a knowledge base.

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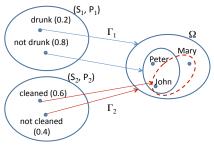
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Murder example continued

- The first item of evidence gave us:  $m_1(\{Peter, John\}) = 0.8$ ,  $m_1(\Omega) = 0.2$ .
- New piece of evidence: a blond hair has been found.
- There is a probability 0.6 that the room has been cleaned before the crime: m<sub>2</sub>({John, Mary}) = 0.6, m<sub>2</sub>(Ω) = 0.4.
- How to combine these two pieces of evidence?

Justification



- If interpretations s<sub>1</sub> ∈ S<sub>1</sub> and s<sub>2</sub> ∈ S<sub>2</sub> both hold, then X ∈ Γ<sub>1</sub>(s<sub>1</sub>) ∩ Γ<sub>2</sub>(s<sub>2</sub>).
- If the two pieces of evidence are independent, then the probability that s<sub>1</sub> and s<sub>2</sub> both hold is P<sub>1</sub>({s<sub>1</sub>})P<sub>2</sub>({s<sub>2</sub>}).
- If Γ<sub>1</sub>(s<sub>1</sub>) ∩ Γ<sub>2</sub>(s<sub>2</sub>) = Ø, we know that s<sub>1</sub> and s<sub>2</sub> cannot hold simultaneously.
- The joint probability distribution on S<sub>1</sub> × S<sub>2</sub> must be conditioned to eliminate such pairs.

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• Let *m*<sub>1</sub> and *m*<sub>2</sub> be two mass functions and

$$\kappa = \sum_{B \cap C = \emptyset} m_1(B) m_2(C)$$

their degree of conflict.

• If K < 1, then  $m_1$  and  $m_2$  can be combined as

$$(m_1 \oplus m_2)(A) = \frac{1}{1-\kappa} \sum_{B \cap C=A} m_1(B)m_2(C), \quad \forall A \neq \emptyset,$$

and  $(m_1 \oplus m_2)(\emptyset) = 0$ .

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## Dempster's rule

**Properties** 

- Commutativity, associativity. Neutral element: m<sub>Ω</sub>.
- Generalization of intersection: if m<sub>A</sub> and m<sub>B</sub> are logical mass functions and  $A \cap B \neq \emptyset$ , then

$$m_A \oplus m_B = m_{A \cap B}$$

- Generalization of probabilistic conditioning: if m is a Bayesian mass function and  $m_A$  is a logical mass function, then  $m \oplus m_A$  is a Bayesian mass function corresponding to the conditioning of m by A.
- Notation for conditioning (special case):

$$m \oplus m_A = m(\cdot | A).$$

 Contour functions: if pl and pl' are the contour functions of m and m', and pl'' is the contour function of  $m'' = m \oplus m'$ , then

$$pl'' \propto pl \cdot pl'$$
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### Decision analysis

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## Problem formulation

- A decision problem can be formalized by defining:
  - A set of acts  $\mathcal{A} = \{a_1, \ldots, a_s\};$
  - A set of states of the world Ω;
  - A loss function L : A × Ω → ℝ, such that L(a, ω) is the loss incurred if we select act a and the true state is ω.
- Bayesian framework
  - Uncertainty on  $\Omega$  is described by a probability measure *P*;
  - Define the risk of each act a as the expected loss if a is selected:

$$R_P(a) = \mathbb{E}_P[L(a, \cdot)] = \sum_{\omega \in \Omega} L(a, \omega) P(\{\omega\}).$$

- Select an act with minimal risk.
- Extension when uncertainty on Ω is described by a belief function?

## Lower and upper risks

• Lower expectation (optimistic):

$$\underline{R}(a) = \sum_{A \subseteq \Omega} m(A) \min_{\omega \in A} L(a, \omega)$$

• Upper expectation (pessimistic):

$$\overline{R}(a) = \sum_{A \subseteq \Omega} m(A) \max_{\omega \in A} L(a, \omega)$$

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## Compromising between the lower and upper risks

Hurwicz criterion:

$$R_{\rho}(a) = (1 - \rho)\underline{R}(a) + 
ho\overline{R}(a),$$

where  $\rho \in [0, 1]$  is a pessimism index describing the attitude of the decision maker in the face of ambiguity.

• Pignistic expectation

$$\begin{aligned} R_{bet}(a) &= \sum_{A \subseteq \Omega} \left( m(A) \frac{1}{|A|} \sum_{\omega \in A} L(a, \omega) \right) \\ &= \sum_{\omega \in \Omega} L(a, \omega) bet p_m(\omega) \end{aligned}$$

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## **Decision strategies**

• Minimization of lower risk (optimistic):

 $a \succeq a' \text{ iff } \underline{R}(a) \leq \underline{R}(a')$ 

Minimization of upper risk (pessimistic):

 $a \succeq a' \text{ iff } \overline{R}(a) \leq \overline{R}(a')$ 

Hurwicz criterion:

$${\pmb{a}} \succeq {\pmb{a}}' ext{ iff } {\pmb{R}}_{
ho}({\pmb{a}}) \leq {\pmb{R}}_{
ho}({\pmb{a}}')$$

Minimization of pignistic risk:

$$a \succeq a' \text{ iff } R_{bet}(a) \leq R_{bet}(a')$$

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## Interval dominance rule

- Act *a* dominates a'  $(a \succeq a')$  if  $\overline{R}(a) \leq \underline{R}(a')$ .
- If the intervals [<u>R</u>(a), <u>R</u>(a)] and [<u>R</u>(a'), <u>R</u>(a')] intersect, a and a' are not comparable. We thus get a partial preorder.
- The interval dominance rule selects the set of non dominated acts (the set of acts *a* such that no act is strictly preferred to *a*)

$$\{a \in \mathcal{A} | \forall a' \in \mathcal{A}, \neg (a' \succ a)\}$$

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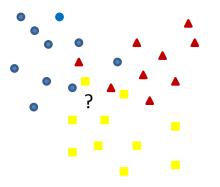
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## **Classification problem**



- A population is assumed to be partitioned in *c* groups or classes
- Let  $\Omega = \{\omega_1, \dots, \omega_c\}$  denote the set of classes
- Each instance is described by
  - A feature vector  $\boldsymbol{x} \in \mathbb{R}^{p}$
  - A class label  $y \in \Omega$
- Problem: given a learning set  $\mathcal{L} = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$ , predict the class label of a new instance described by  $\mathbf{x}$

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### Dempster-Shafer theory

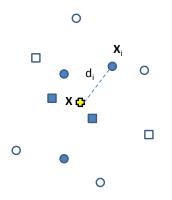
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# Evidential classification Evidential K-NN rule

- Evidential neural network classifier
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## **Principle**



- Let N<sub>K</sub>(x) ⊂ L denote the set of the K nearest neighbors of x in L, based on some distance measure
- Each *x<sub>i</sub>* ∈ *N<sub>K</sub>*(*x*) can be considered as a piece of evidence regarding the class of *x*
- The strength of this evidence decreases with the distance *d<sub>i</sub>* between *x* and *x<sub>i</sub>*

## Definition

• If  $y_i = \omega_k$ , the evidence of  $(\mathbf{x}_i, y_i)$  can be represented by

$$\begin{split} m_i(\{\omega_k\}) &= \varphi_k\left(d_i\right) \\ m_i(\{\omega_\ell\}) &= 0, \quad \forall \ell \neq k \\ m_i(\Omega) &= 1 - \varphi\left(d_i\right) \end{split}$$

where  $\varphi_k$ , k = 1, ..., c are decreasing functions from  $[0, +\infty)$  to [0, 1] such that  $\lim_{d \to +\infty} \varphi_k(d) = 0$ 

• The evidence of the *K* nearest neighbors of *x* is pooled using Dempster's rule of combination

$$m = \bigoplus_{\boldsymbol{x}_i \in \mathcal{N}_{\mathcal{K}}(\boldsymbol{x})} m_i$$

- Decision: any of the decision rules mentioned in the first part.
- With 0-1 losses and no rejection, the optimistic, pessimistic and pignistic rules yield the same decisions.

## Learning

- Choice of functions  $\varphi_k$ : for instance,  $\varphi_k(d) = \alpha \exp(-\gamma_k d^2)$ .
- Parameters  $\gamma_1, \ldots, \gamma_c$  can be optimized (see below).
- Parameter γ = (γ<sub>1</sub>,..., γ<sub>c</sub>) can be learnt from the data by minimizing the following cost function

$$\mathcal{C}(\boldsymbol{\gamma}) = \sum_{i=1}^n \sum_{k=1}^c (\mathcal{p}l_{(-i)}(\omega_k) - t_{ik})^2,$$

where

- *pl*<sub>(-*i*)</sub> is the contour function obtained by classifying **x**<sub>*i*</sub> using its *K* nearest neighbors in the learning set.
- $t_{ik} = 1$  is  $y_i = k$ ,  $t_{ik} = 0$  otherwise.
- Function C(γ) can be minimized by an iterative nonlinear optimization algorithm.

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## Computation of $pl_{(-i)}$

• Contour function from each neighbor  $\mathbf{x}_j \in \mathcal{N}_{\mathcal{K}}(\mathbf{x}_i)$ :

$$\mathcal{p}l_j(\omega_k) = egin{cases} 1 & ext{if } y_j = \omega_k \ 1 - arphi_k(d_{ij}) & ext{otherwise} \end{cases}, \quad k = 1, \dots, c$$

Contour function of the combined mass function

$$\mathcal{P}l_{(-i)}(\omega_k) \propto \prod_{oldsymbol{x}_j \in \mathcal{N}_{\mathcal{K}}(oldsymbol{x}_i)} \left(1 - arphi_k(oldsymbol{d}_{ij})
ight)^{1 - t_{jk}}$$

where  $t_{jk} = 1$  if  $y_j = \omega_k$  and  $t_{jk} = 0$  otherwise

It can be computed in time proportional to K|Ω|

## Example 1: Vehicles dataset

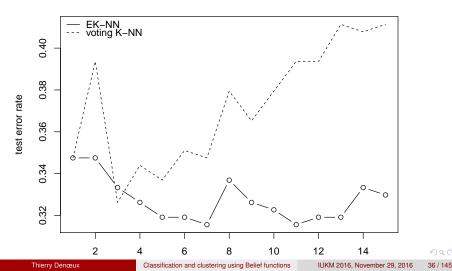
- The data were used to distinguish 3D objects within a 2-D silhouette of the objects.
- Four classes: bus, Chevrolet van, Saab 9000 and Opel Manta.
- 846 instances, 18 numeric attributes.
- The first 564 objects are training data, the rest are test data.

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## Vehicles datasets: result

### Vehicles data



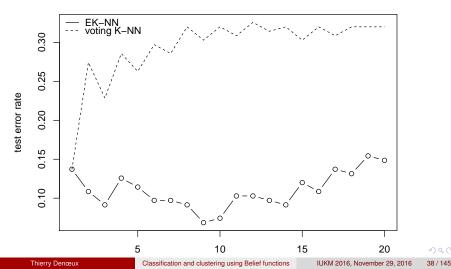
### Example 2: Ionosphere dataset

- This dataset was collected by a radar system and consists of phased array of 16 high-frequency antennas with a total transmitted power of the order of 6.4 kilowatts.
- The targets were free electrons in the ionosphere. "Good" radar returns are those showing evidence of some type of structure in the ionosphere. "Bad" returns are those that do not.
- There are 351 instances and 34 numeric attributes. The first 175 instances are training data, the rest are test data.

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### lonosphere datasets: result

#### **lonosphere** data



### Implementation in R

```
library("evclass")
```

```
data("ionosphere")
xapp<-ionosphere$x[1:176,]
yapp<-ionosphere$y[1:176]
xtst<-ionosphere$x[177:351,]
ytst<-ionosphere$y[177:351]</pre>
```

```
opt<-EkNNfit(xapp,yapp,K=10)
class<-EkNNval(xapp,yapp,xtst,K=10,ytst,opt$param)</pre>
```

```
> class$err
0.07428571
> table(ytst,class$ypred)
ytst 1 2
1 106 6
2 7 56
```

### Partially supervised data

• We now consider a learning set of the form

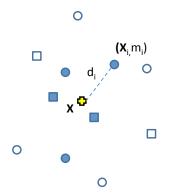
$$\mathcal{L} = \{(\boldsymbol{x}_i, m_i), i = 1, \ldots, n\}$$

where

- **x**<sub>*i*</sub> is the attribute vector for instance *i*, and
- *m<sub>i</sub>* is a mass function representing uncertain expert knowledge about the class *y<sub>i</sub>* of instance *i*
- Special cases:
  - $m_i(\{\omega_k\}) = 1$  for all *i*: supervised learning
  - $m_i(\Omega) = 1$  for all *i*: unsupervised learning

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### Evidential k-NN rule for partially supervised data



• Each mass function *m<sub>i</sub>* is discounted (weakened) with a rate depending on the distance *d<sub>i</sub>* 

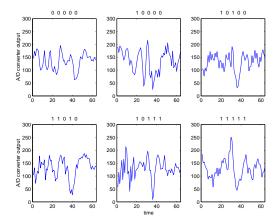
$$egin{aligned} m_i'(m{A}) &= arphi\left(m{d}_i
ight) m_i(m{A}), & orall m{A} \subset \Omega \ m_i'(\Omega) &= 1 - \sum_{m{A} \subset \Omega} m_i'(m{A}) \end{aligned}$$

• The *K* mass functions *m*<sup>'</sup><sub>i</sub> are combined using Dempster's rule

$$m = \bigoplus_{\boldsymbol{x}_i \in \mathcal{N}_{\mathcal{K}}(\boldsymbol{x})} m'_i$$

### Example: EEG data

EEG signals encoded as 64-D patterns, 50 % positive (K-complexes), 50 % negative (delta waves), 5 experts.



## Results on EEG data

(Denoeux and Zouhal, 2001)

- *c* = 2 classes, *p* = 64
- For each learning instance **x**<sub>i</sub>, the expert opinions were modeled as a mass function *m*<sub>i</sub>.
- n = 200 learning patterns, 300 test patterns

K	<i>K</i> -NN	w K-NN	Ev. K-NN	Ev. K-NN
			(crisp labels)	(uncert. labels)
9	0.30	0.30	0.31	0.27
11	0.29	0.30	0.29	0.26
13	0.31	0.30	0.31	0.26

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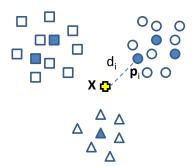
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### Principle



- The learning set is summarized by r prototypes.
- Each prototype *p<sub>i</sub>* has membership degree  $u_{ik}$  to each class  $\omega_k$ , with  $\sum_{k=1}^{c} u_{ik} = 1.$
- Each prototype  $p_i$  is a piece of evidence about the class of x, whose reliability decreases with the distance  $d_i$  between  $\boldsymbol{x}$  and  $\boldsymbol{p}_i$ .

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### Propagation equations

Mass function induced by prototype p<sub>i</sub>:

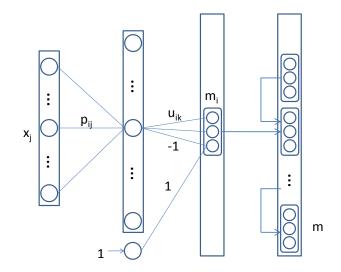
$$m_i(\{\omega_k\}) = \alpha_i u_{ik} \exp(-\gamma_i d_i^2), \quad k = 1, \dots, c$$
$$m_i(\Omega) = 1 - \alpha_i \exp(-\gamma_i d_i^2)$$

Combination:

$$m=\bigoplus_{i=1}^r m_i$$

- The computation of  $m_i$  requires O(rp) arithmetic operations (where p denotes the number of inputs), and the combination can be performed in O(rc) operations. Hence, the overall complexity is O(r(p+c)) operations to compute the output for one input pattern.
- The combined mass function *m* has as focal sets the singletons  $\{\omega_k\}$ ,  $k = 1, \ldots, c$  and  $\Omega$ .

### Neural network implementation



### Learning

- The parameters are the
  - The prototypes  $\boldsymbol{p}_i$ , i = 1, ..., r (*rp* parameters)
  - The membership degrees  $u_{ik}$ , i = 1, ..., r, k = 1, ..., c (*rc* parameters)
  - The  $\alpha_i$  and  $\gamma_i$ ,  $i = 1 \dots, r$  (2*r* parameters).
- Let θ denote the vector of all parameters. It can be estimated by minimizing a cost function such as

$$\mathcal{C}(\boldsymbol{ heta}) = \sum_{i=1}^{n} (\mathcal{P}l_{ik} - t_{ik})^2 + \mu \sum_{i=1}^{r} lpha_{ik}$$

where  $pl_{ik}$  is the output plausibility for instance *i* and class *k*,  $t_{ik} = 1$  if  $y_i = k$  and  $t_{ik} = 0$  otherwise, and  $\mu$  is a regularization coefficient (hyperparameter).

• The hyperparameter  $\mu$  can be optimized by cross-validation.

### Implementation in R

```
library("evclass")
```

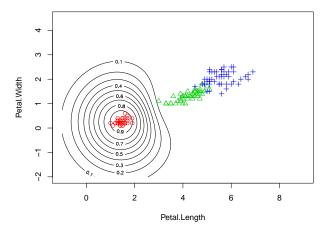
```
data(glass)
xtr<-glass$x[1:89,]
ytr<-glass$y[1:89]
xtst<-glass$x[90:185,]
vtst<-glass$v[90:185]</pre>
```

```
param0<-proDSinit(xtr,ytr,nproto=7)
fit<-proDSfit(x=xtr,y=ytr,param=param0)
val<-proDSval(xtst,fit$param,ytst)</pre>
```

```
> print(val$err)
0.3333333 > table(ytst,val$ypred)
ytst 1 2 3 4
1 30 6 4 0
2 6 27 1 3
3 4 3 1 0
4 0 5 0 6
```

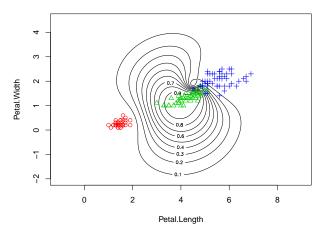
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Mass on  $\{\omega_1\}$ 



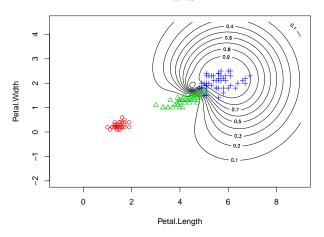
m({ω<sub>1</sub>})

Mass on  $\{\omega_2\}$ 



 $m(\{\omega_2\})$ 

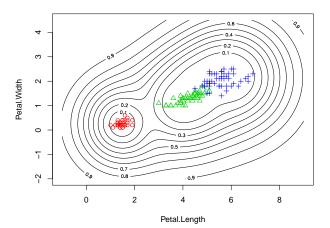
Mass on  $\{\omega_3\}$ 



m({ω<sub>3</sub>})

= 200

Mass on  $\Omega$ 

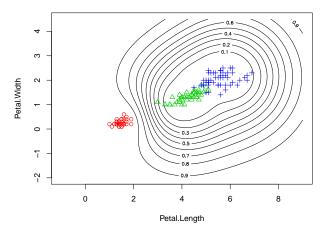


 $m(\Omega)$ 

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Plausibility of  $\{\omega_1\}$ 

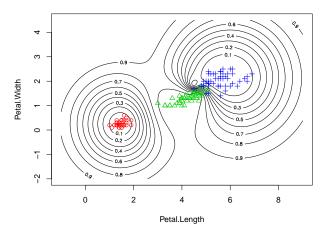


 $PI(\{\omega_1\})$ 

= 200

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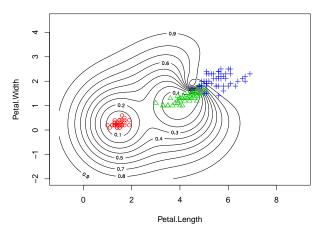
Plausibility of  $\{\omega_2\}$ 



 $PI(\{\omega_2\})$ 

= 990

Plausibility of  $\{\omega_3\}$ 



 $PI(\{\omega_3\})$ 

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= 990

### Outline

#### Dempster-Shafer theory

- Mass, belief and plausibility functions
- Dempster's rule
- Decision analysis

#### Evidential classification

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#### Evidential clustering

- Evidential partition
- Evidential c-means
- EVCLUS
- Ek-NNclus

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### Simple decision setting

• To formalize the decision problem, we need to define:

- The acts
- The loss matrix
- For instance, let the acts be
  - $a_k$  = assignment to class  $\omega_k$ ,  $k = 1, \ldots, c$
- And the loss matrix (for *c* = 3)

	<i>a</i> 1	$a_2$	$a_3$
$\omega_1$	0	1	1
$\omega_2$	1	0	1
$\omega_3$	1	1	0

- $\underline{R}(a_i) = 1 Pl(\{\omega_i\})$  and  $\overline{R}(a_i) = 1 Bel(\{\omega_i\})$ .
- The optimistic, pessimistic and pignistic decision rules yield the same result

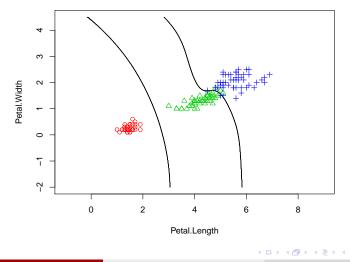
### Implementation in R

```
param0<-proDSinit(x,y,6)
fit<-proDSfit(x,y,param0)</pre>
```

```
val<-proDSval(xtst,fit$param)
L<-1-diag(c)
D<-decision(val$m,L=L,rule='upper')</pre>
```

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### Decision with rejection

#### Let the acts now be

- $a_k$  = assignment to class  $\omega_k$ ,  $k = 1, \ldots, c$
- $a_0$  = rejection
- And the loss matrix (for *c* = 3)

	a <sub>1</sub>	$a_2$	$a_3$	$a_0$
$\omega_1$	0	1	1	$\lambda_0$
$\omega_2$	1	0	1	$\lambda_0$
$\omega_3$	1	1	0	$\lambda_0$

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### Implementation in R

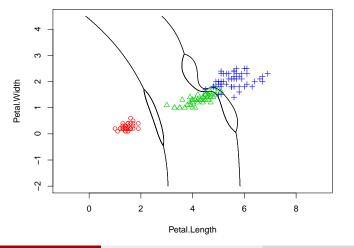
```
param0<-proDSinit(x,y,6)
fit<-proDSfit(x,y,param0)</pre>
```

```
val<-proDSval(xtst,fit$param)
L<-cbind(1-diag(c),rep(0.3,c))
D1<-decision(val$m,L=L,rule='upper')
D2<-decision(val$m,L=L,rule='lower')
D3<-decision(val$m,L=L,rule='pignistic')
D4<-decision(val$m,L=L,rule='hurwicz',rho=0.5)</pre>
```

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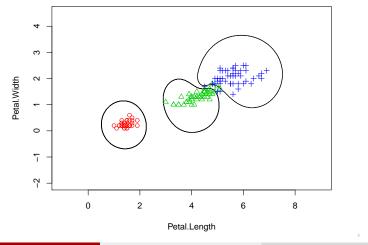
Lower risk



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Classification and clustering using Belief functions

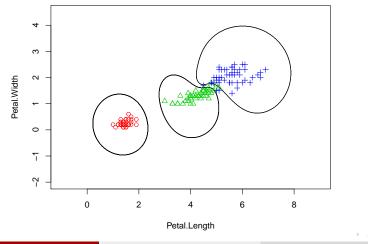
Upper risk



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Classification and clustering using Belief functions

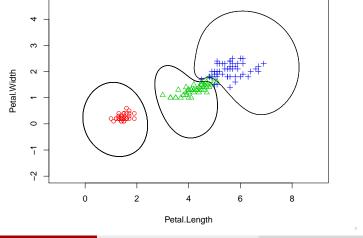
Pignistic risk



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Classification and clustering using Belief functions

Hurwicz strategy ( $\rho = 0.5$ )



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Classification and clustering using Belief functions

### Decision with rejection and novelty detection

- Assume that there exists an unknown class ω<sub>u</sub>, not represented in the learning set
- Let the acts now be
  - $a_k$  = assignment to class  $\omega_k$ ,  $k = 1, \ldots, c$
  - $a_u$  = assignment to class  $\omega_u$
  - $a_0 =$  rejection
- And the loss matrix

	a <sub>1</sub>	$a_2$	$a_3$	$a_0$	$a_u$
$\omega_1$	0	1	1	$\lambda_0$	$\lambda_u$
$\omega_2$	1	0	1	$\lambda_0$	$\lambda_u$
$\omega_3$	1	1	0	$\lambda_0$	$\lambda_u$
$\omega_u$	1	1	1	$\lambda_0$	0

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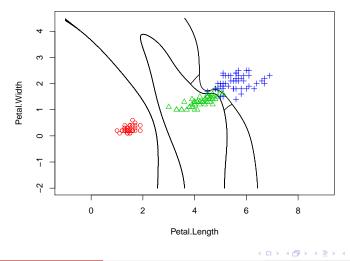
### Implementation in R

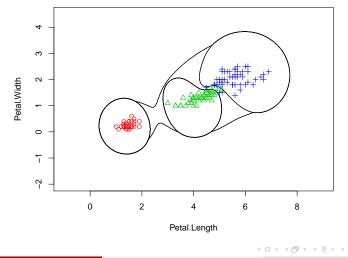
```
param0<-proDSinit(x,y,6)
fit<-proDSfit(x,y,param0)</pre>
```

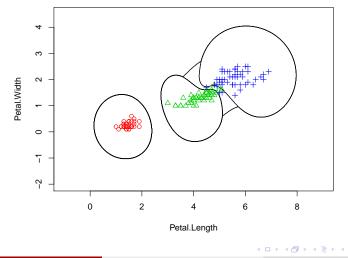
```
val<-proDSval(xtst,fit$param)
L<-cbind(1-diag(c),rep(0.3,c),rep(0.32,c))
L<-rbind(L,c(1,1,1,0.3,0))
D1<-decision(val$m,L=L,rule='lower')
D2<-decision(val$m,L=L,rule='pignistic')
D3<-decision(val$m,L=L,rule='hurwicz',rho=0.5)</pre>
```

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### References on classification I

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

### T. Denœux.

A k-nearest neighbor classification rule based on Dempster-Shafer theory.

IEEE Transactions on SMC, 25(05):804-813, 1995.

#### T. Denœux.

A neural network classifier based on Dempster-Shafer theory. IEEE transactions on SMC A, 30(2):131–150, 2000.

### T. Denœux.

Analysis of evidence-theoretic decision rules for pattern classification. Pattern Recognition, 30(7):1095–1107, 1997.

#### C. Lian, S. Ruan and T. Denœux.

An evidential classifier based on feature selection and two-step classification strategy.

Pattern Recognition, 48:2318–2327, 2015.

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## References on classification II

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

C. Lian, S. Ruan and T. Denœux.
 Dissimilarity metric learning in the belief function framework.
 IEEE Transactions on Fuzzy Systems (to appear), 2016.

## Outline

#### Dempster-Shafer theory

- Mass, belief and plausibility functions
- Dempster's rule
- Decision analysis

#### Evidential classification

- Evidential K-NN rule
- Evidential neural network classifier
- Decision analysis

## Evidential clustering

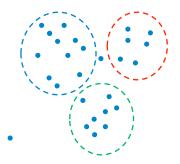
- Evidential partition
- Evidential *c*-means
- EVCLUS

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## Clustering



- n objects described by
  - Attribute vectors *x*<sub>1</sub>,..., *x<sub>n</sub>* (attribute data) or
  - Dissimilarities (proximity data).
- Goals:
  - Discover groups in the data;
  - 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.

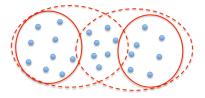
Fuzzy clustering with noise cluster: the above equality is replaced by  $\sum_{k=1}^{c} u_{ik} \leq 1$ . The number  $1 - \sum_{k=1}^{c} u_{ik}$  is interpreted as a degree of membership (or probability of belonging to) to a noise cluster.

## 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  $\omega_k$  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.

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  - Evidential K-NN rule
  - Evidential neural network classifier
  - Decision analysis

## Evidential clustering

- Evidential partition
- Evidential *c*-means
- EVCLUS
- E*k*-NNclus

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# **Clustering concepts**

Hard and fuzzy clustering

- Hard clustering: each object belongs to one and only one group. Group membership is expressed 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  $\sum_{k=1}^{c} u_{ik} = 1$
- Fuzzy clustering with noise cluster: each object has a degree of membership u<sub>ik</sub> ∈ [0, 1] to each group and a degree of membership u<sub>i\*</sub> ∈ [0, 1] to a noise cluster, with ∑<sub>k=1</sub><sup>c</sup> u<sub>ik</sub> + u<sub>i\*</sub> = 1

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# **Clustering concepts**

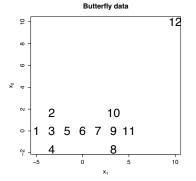
Possibilistic, rough, credal clustering

- Possibilistic clustering: the condition  $\sum_{k=1}^{c} u_{ik} = 1$  is relaxed. Each number  $u_{ik}$  can be interpreted as a degree of possibility that object *i* belongs to cluster *k*
- Rough clustering: the membership of object *i* to cluster *k* is described by a pair  $(\underline{u}_{ik}, \overline{u}_{ik}) \in \{0, 1\}^2$ , with  $\underline{u}_{ik} \leq \overline{u}_{ik}$ , indicating its membership to the lower and upper approximations of cluster *k*
- Evidential clustering: based on Dempster-Shafer (DS) theory (the topic of this talk)

#### Evidential partition

## Evidential clustering

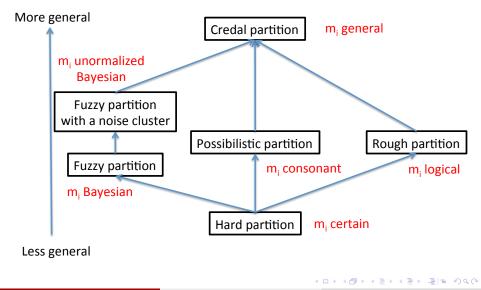
- In evidential clustering, the cluster membership of each object is considered to be uncertain and is described by a (not necessarily normalized) mass function  $m_i$  over  $\Omega$
- The *n*-tuple  $\mathcal{M} = (m_1, \ldots, m_n)$  is called a credal partition
- Example:



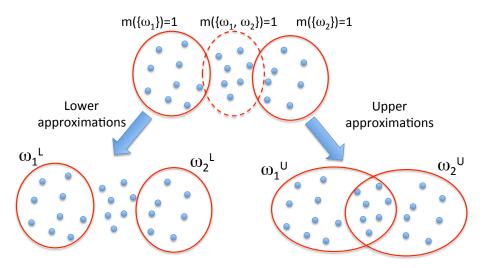
Credal partition						
	Ø	$\{\omega_1\}$	$\{\omega_2\}$	$\{\omega_1, \omega_2\}$		
$m_3$	0	1	0	0		
$m_5$	0	0.5	0	0.5		
$m_6$	0	0	0	1		
$m_{12}$	0.9	0	0.1	0		

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## Relationship with other clustering structures

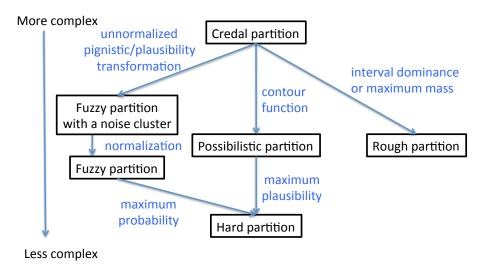


## Rough clustering as a special case



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## Summarization of a credal partition



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## From evidential to rough clustering

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

$$\mathbf{A}_{i} = \{ \omega \in \Omega | \forall \omega' \in \Omega, \mathbf{Bel}_{i}^{*}(\{\omega'\}) \leq \mathbf{Pl}_{i}^{*}(\{\omega\}) \},\$$

where *Bel*<sup>\*</sup> and *Pl*<sup>\*</sup> 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:

$$\overline{u}_{ik} = egin{cases} 1 & ext{if } \omega_k \in \mathcal{A}_i \ 0 & ext{otherwise.} \end{cases}$$

• The outliers can be identified separately as the objects for which  $m_i(\emptyset) \ge m_i(A)$  for all  $A \ne \emptyset$ .

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## Algorithms

Evidential c-means (ECM): (Masson and Denoeux, 2008):

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

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#### Evidential c-means

## Outline

#### Dempster-Shafer theory

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### Evidential clustering

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- Evidential c-means
- EVCLUS

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## **Principle**

- Problem: generate a credal partition  $M = (m_1, ..., m_n)$  from attribute data  $X = (\mathbf{x}_1, ..., \mathbf{x}_n), \mathbf{x}_i \in \mathbb{R}^p$ .
- 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.

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## Fuzzy c-means (FCM)

Minimize

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

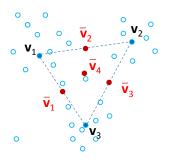
with  $d_{ik} = ||\mathbf{x}_i - \mathbf{v}_k||$  subject to the constraints  $\sum_k u_{ik} = 1$  for all *i*.

Alternate optimization algorithm:

$$\mathbf{v}_{k} = \frac{\sum_{i=1}^{n} u_{ik}^{\beta} \mathbf{x}_{i}}{\sum_{i=1}^{n} u_{ik}^{\beta}}$$
$$u_{ik} = \frac{d_{ik}^{-2/(\beta-1)}}{\sum_{\ell=1}^{c} d_{i\ell}^{-2/(\beta-1)}}.$$

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# ECM algorithm



- Each cluster  $\omega_k$  represented by a prototype  $\boldsymbol{v}_k$ .
- Basic ideas:
  - For each nonempty A<sub>j</sub> ∈ Ω, m<sub>ij</sub> = m<sub>i</sub>(A<sub>j</sub>) should be high if x<sub>i</sub> is close to v
    <sub>j</sub>.
  - The distance to the empty set is defined as a fixed value  $\delta$ .

## ECM algorithm: objective criterion

- Define the nonempty focal sets F = {A<sub>1</sub>,..., A<sub>f</sub>} ⊆ 2<sup>Ω</sup> \ {∅}.
- Minimize

$$J_{ ext{ecm}}(M,V) = \sum_{i=1}^n \sum_{j=1}^f |A_j|^lpha m_{ij}^eta d_{ij}^2 + \sum_{i=1}^n \delta^2 m_{i\emptyset}^eta$$

subject to the constraints  $\sum_{j=1}^{f} m_{ij} + m_{i\emptyset} = 1$  for all *i*.

- Parameters:
  - $\alpha$  controls the specificity of mass functions (default: 1)
  - $\beta$  controls the hardness of the credal partition (default: 2)
  - $\delta$  controls the proportion of data considered as outliers

•  $J_{ECM}(M, V)$  can be iteratively minimized with respect to M and to V.

## ECM algorithm: update equations

Update of *M*:

$$m_{ij} = \frac{c_j^{-\alpha/(\beta-1)} d_{ij}^{-2/(\beta-1)}}{\sum_{k=1}^{f} c_k^{-\alpha/(\beta-1)} d_{ik}^{-2/(\beta-1)} + \delta^{-2/(\beta-1)}},$$
  
for  $i = 1, \dots, n$  and  $j = 1, \dots, f$ , and  
 $m_{i\emptyset} = 1 - \sum_{j=1}^{f} m_{ij}, \quad i = 1, \dots, n$ 

Update of *V*: solve a linear system of the form

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where *B* is a matrix of size  $c \times p$  and *H* a matrix of size  $c \times c$ .

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## Implementation in R

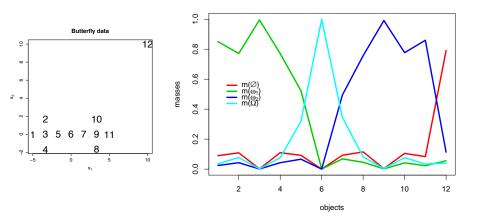
```
library(evclust)
data('butterfly')
n<-nrow(butterfly)</pre>
```

```
clus<-ecm(butterfly[,1:2],c=2,delta=sqrt(20))</pre>
```

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## Butterfly dataset



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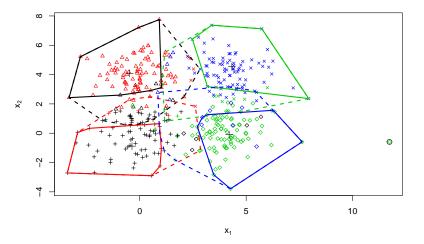
## Four-class dataset

```
data("fourclass")
clus<-ecm(fourclass[,1:2],c=4,type='pairs',delta=5)</pre>
```

plot(clus,X=fourclass[,1:2],ytrue=fourclass[,3],Outliers = TRUE,
approx=2)

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## 4-class data set



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## Handling a large number of clusters

- If no restriction is imposed on the focal sets, the number of parameters to be estimated in evidential clustering grows exponentially with the number *c* of clusters, which makes it intractable unless *c* is small.
- If we allow masses to be assigned to all pairs of clusters, the number of focal sets becomes proportional to  $c^2$ , which is manageable for moderate values of c (say, until 10), but still impractical for larger n.
- Idea: assign masses only to pairs of contiguous clusters.

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## Method

- In the first step, ECM is run in the basic configuration, with focal sets of cardinalities 0, 1 and (optionally) c. A credal partition M<sub>0</sub> is obtained.
- 2 The similarity between each pair of clusters  $(\omega_j, \omega_\ell)$  is computed as

$$S(j, \ell) = \sum_{i=1}^{n} \rho I_{ij} \rho I_{i\ell},$$

where  $p_{lj}$  and  $p_{l\ell}$  are the normalized plausibilities that object *i* belongs, respectively, to clusters *j* and  $\ell$ . We then determine the set  $P_K$  of pairs  $\{\omega_j, \omega_\ell\}$  that are mutual *K* nearest neighbors.

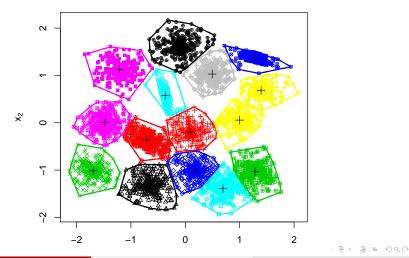
Section 8 ECM is run again, starting from the previous evidential partition  $\mathcal{M}_0$ , and adding as focal sets the pairs in  $P_{\mathcal{K}}$ .

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## Example in R: step 1

data(s2)
clus<-ecm(x=s2,c=15,type='simple',Omega=FALSE,delta=1,disp=FALSE)
plot(x=clus,X=s2,Outliers = TRUE)</pre>

## **Result after Step 1**



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Classification and clustering using Belief functions

## Example in R: steps 2 and 3

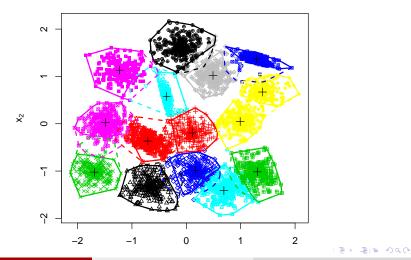
```
P<-createPairs(clus,k=2)</pre>
```

```
clus1<-ecm(x=s2,c=15,type='pairs',Omega=FALSE,pairs=P$pairs,
g0=clus$g,delta=1,disp=FALSE)
```

```
plot(x=clus1, X=s2, Outliers = TRUE, approx=2)
```

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## Final result



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## 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 Ø.
- Nonspecificity of a mass function:

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

• Proposed validity index of a credal partition:

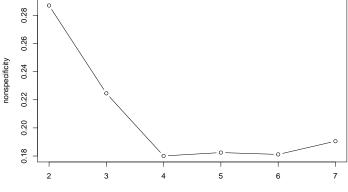
$$N^*(c) \triangleq rac{1}{n \log_2(c)} \sum_{i=1}^n \left[ \sum_{A \in 2^\Omega \setminus \emptyset} m_i(A) \log_2 |A| + m_i(\emptyset) \log_2(c) 
ight]$$

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## Example (Four-class dataset)

```
C<-2:7
N<-rep(0,length(C))
for(k in 1:length(C)){
clus<-ecm(fourclass[,1:2],c=C[k],type='pairs',alpha=2,
delta=5,disp=FALSE)
N[k]<-clus$N
}
plot(C,N,type='b',xlab='c',ylab='nonspecificity')
```

## Results for the 4-class dataset



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## 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:
  - Must-link (ML) constraints, which specify that two objects certainly belong to the same cluster;
  - Cannot-link (CL) constraints, which specify that two objects certainly belong to different clusters.
- How to take into account such constraints?

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## Modified cost-function

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

$$J_{ ext{cecm}}(M,V) = (1-\xi)J_{ ext{ecm}}(M,V) + \xi J_{ ext{const}}(M)$$

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<sub>ij</sub>(S)* and *pl<sub>ij</sub>(¬S)* are computed from the pairwise mass function *m<sub>ij</sub>* Go back to pairwise mass functions
- Minimizing  $J_{CECM}(M, V)$  w.r.t. *M* is a quadratic programming problem.

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#### Evidential c-means

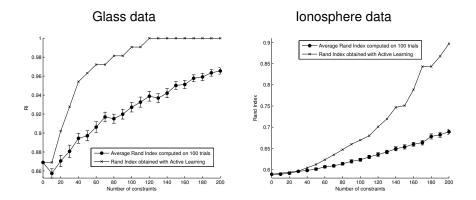
## Active learning

- 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.

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#### **Results**



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### 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

- Evidential K-NN rule
- Evidential neural network classifier
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#### Evidential clustering

- Evidential partition
- EVCLUS

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## 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?

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## Formalization

- Let m<sub>i</sub> and m<sub>i</sub> be mass functions regarding the group membership of objects  $o_i$  and  $o_i$ .
- The plausibility of the proposition  $S_{ij}$ : "objects  $o_i$  and  $o_j$  belong to the same group" can be shown to be equal to:

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

where  $\kappa_{ii} = \text{degree of conflict}$  between  $m_i$  and  $m_i$ .

• Problem: find a credal partition  $M = (m_1, \ldots, m_n)$  such that larger degrees of conflict  $\kappa_{ii}$  correspond to larger dissimilarities  $d_{ii}$ .

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## Cost function

- Approach: minimize the discrepancy between the dissimilarities  $d_{ii}$  and the degrees of conflict  $\kappa_{ii}$ .
- Example of a cost (stress) function:

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

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

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

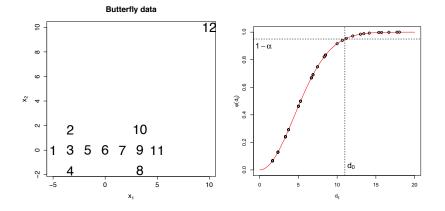
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## Butterfly example

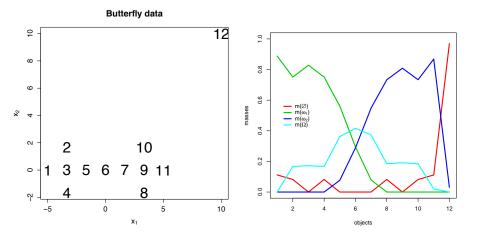
Data and dissimilarities

Determination of  $\gamma$  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  $d_{ij} \ge d_0$ , the plausibility that they belong to the same cluster is at least  $1 - \alpha$ .



# Butterfly example

Credal partition

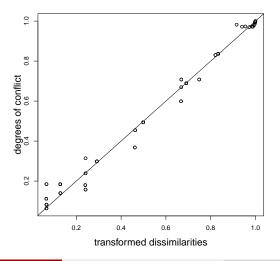


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# Butterfly example

Shepard diagram



Classification and clustering using Belief functions

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## Optimization algorithm

- How to minimize J(M)? Two methods:
  - Using a gradient descent or quasi-Newton algorithm (slow).
  - Substitution Using a cyclic coordinate descent algorithm minimizing J(M) with respect to each  $m_i$  at a time.
- The latter approach exploits the particular approach of the problem (a quadratic programming problem is solved at each step), and it is thus much more efficient.

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## Implementation in R

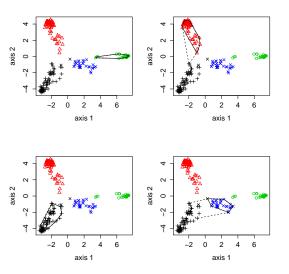
```
library(evclust)
data(protein)
```

clus <- kevclus(D=protein\$D,c=4,type='simple',d0=max(protein\$D))</pre>

```
z<- cmdscale(protein$D,k=2)</pre>
```

```
plot(clus,X=z,mfrow=c(2,2),ytrue=protein$y,
Outliers=FALSE,approx=1)
```

#### Proteins data



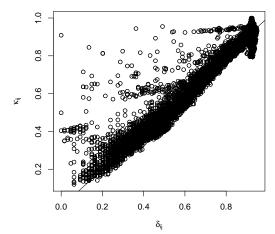
- Nonmetric dissimilarity matrix derived from the structural comparison of 213 protein sequences.
- Ground truth: 4 classes of globins.
- Only 2 errors.

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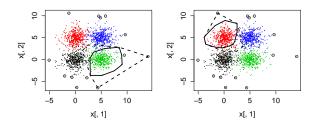
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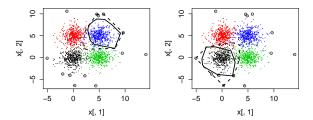
## Proteins data: Shepard diagram



Shepard diagram

### Example with a four-class dataset (2000 objects)





Classification and clustering using Belief functions

## Handling large datasets

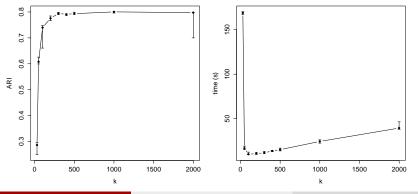
- EVCLUS requires to store the whole dissimilarity matrix: it is inapplicable to large proximity data.
- Idea: compute the differences between degrees of conflict and dissimilarities, for only a subset of randomly sampled dissimilarities.
- Let  $j_1(i), \ldots, j_k(i)$  be *k* integers sampled at random from the set  $\{1, \ldots, i-1, i+1, \ldots, n\}$ , for  $i = 1, \ldots, n$ . Let  $J_k$  the following stress criterion,

$$J_{k}(M) = \sum_{i=1}^{n} \sum_{r=1}^{k} (\kappa_{i,j_{r}(i)} - \delta_{i,j_{r}(i)})^{2}.$$

- The calculation of  $J_k(M)$  requires only O(nk) operations.
- If *k* can be kept constant as *n* increases, then time and space complexity is reduced from quadratic to linear.

## Zongker Digit dissimilarity data

- Similarities between 2000 handwritten digits in 10 classes, based on deformable template matching.
- k-EVCLUS was run with c = 10 and different values of k.
- Parameter d<sub>0</sub> was fixed to the 0.3-quantile of the dissimilarities.
- k-EVCLUS was run 10 times with random initializations.



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#### Outline

#### Dempster-Shafer theory

- Mass, belief and plausibility functions
- Dempster's rule
- Decision analysis

#### Evidential classification

- Evidential K-NN rule
- Evidential neural network classifier
- Decision analysis

#### Evidential clustering

- Evidential partition
- Evidential *c*-means
- EVCLUS

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### Reasoning in the space of all partitions

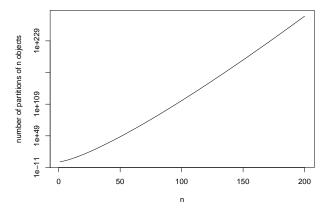
- Assuming there is a true unknown partition, our frame of discernment should be the set *R* of all equivalent relations (≡ partitions) of the set of *n* objects.
- But this set is huge!

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# Number of partitions of *n* objects





Can we implement evidential reasoning in such a large space?

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### Model

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

$$egin{aligned} m_{ij}(\{m{S}\}) &= arphi(m{d}_{ij}), \ m_{ij}(\Theta) &= 1 - arphi(m{d}_{ij}) \end{aligned}$$

where  $\varphi$  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?

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#### Ek-NNclus

### Evidence combination

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

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

- 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  $R \in \mathcal{R}$ .

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#### 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 (E*k*-NN) rule as a base classifier.

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#### Ek-NNclus

#### Example Toy dataset



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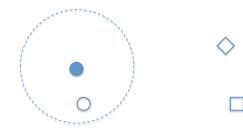
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#### Example Iteration 1

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#### Example Iteration 1 (continued)

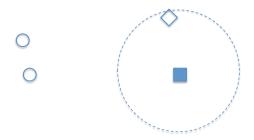


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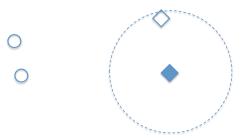
#### Ek-NNclus

#### Example Iteration 2



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#### Example Iteration 2 (continued)



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#### Example Result



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### 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).</li>
- Implementation details:
  - Number *k* of neighbors: two to three times  $\sqrt{n}$ .
  - φ(d) = 1 − exp(−γd<sup>2</sup>), with γ fixed to the inverse of the *q*-quantile of the distances d<sup>2</sup><sub>ii</sub> between an object and its k NN. Typically, q ≥ 0.5.
  - The number of clusters does not need to be fixed in advance.

#### Ek-NNclus

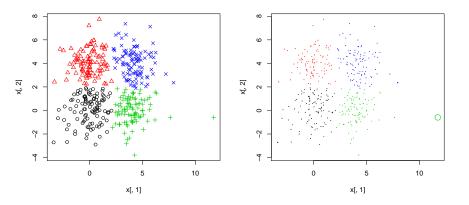
## Ek-NNclus in R

```
data(fourclass)
x<-fourclass[,1:2]
n<-nrow(x)
v0<-1:n
clus < -EkNNclus(x, D, K=50, y0, ntrials = 1, q = 0.5, p = 1)
```

```
plot(x[,1],x[,2],pch=clus$y.pl,col=clus$y.pl)
```

```
c<-ncol(clus$mass)-1
plot(x[,1],x[,2],pch=clus$y,col=clus$y.pl,
cex=0.1+2*clus$mass[,c+1])
```

## Example



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### References on clustering I

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

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#### Summary

- The theory of belief function has great potential in data analysis and challenging machine learning:
  - Classification (supervised learning)
  - Clustering (unsupervised learning) problems
- Belief functions allow us to:
  - Learn from weak information (partially supervised learning, imprecise and uncertain data)
  - Express uncertainty on the outputs of a learning system (e.g., credal partition)
  - Combine the outputs from several learning systems (ensemble classification and clustering), or combine data with expert knowledge (constrained clustering)
- R packages evclass and evclust available from CRAN at https://cran.r-project.org/web/packages

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#### The evclass package

evclass: Evidential Distance-Based Classification

Different evidential distance-based classifiers, which provide outputs in the form of Dempster-Shafer mass functions. The methods are: the evidential K-nearest neighbor rule and the evidential neural network.

Version:	1.1.0	
Depends:	R (≥ 3.1.0)	
Imports:	<u>FNN</u>	
Suggests:	knitr, rmarkdown, datasets	
Published:	2016-07-01	
Author:	Thierry Denoeux	
Maintainer:	Thierry Denoeux <tdenoeux at="" utc.fr=""></tdenoeux>	
License:	<u>GPL-3</u>	
NeedsCompilation: no		
In views:	MachineLearning	
CRAN checks:	evclass results	
Downloads:		
Reference manual:	evclass.pdf	
Vignettes:	Introduction to the evclass package	
Package source:	evclass 1.1.0.tar.gz	
Windows binaries:	r-devel: evclass 1.1.0.zip, r-release: evclass 1.1.0.zip, r-oldrel: evclass 1.1.0.zip	
OS X Mavericks binaries: r-release: evclass 1.1.0.tgz, r-oldrel: evclass 1.1.0.tgz		
Old sources:	evclass archive	

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#### 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:	<u>knitr, rmarkdown</u>	
Published:	2016-09-04	
Author:	Thierry Denoeux	
Maintainer:	Thierry Denoeux <tdenoeux at="" utc.fr=""></tdenoeux>	
License:	GPL-3	
NeedsCompilation: no		
In views:	Cluster	
CRAN checks:	evclust results	

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