Soft clustering: a review of k-means variants

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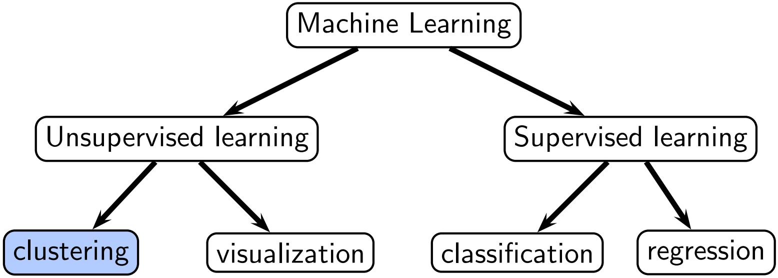
Clustering : a technique of Machine Learning



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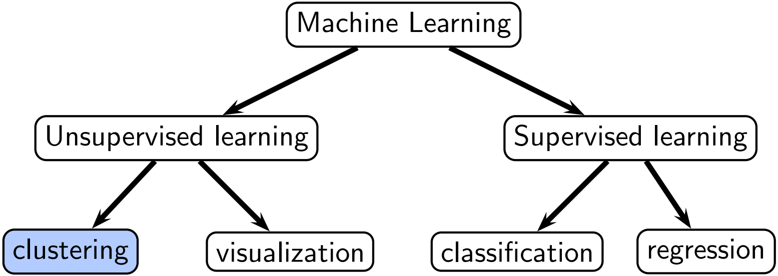
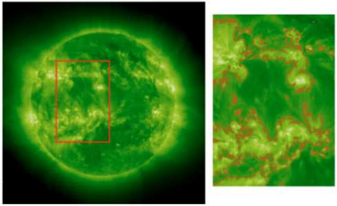


Astronomy [1]



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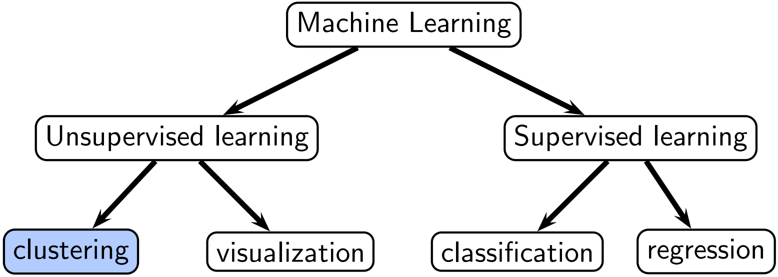

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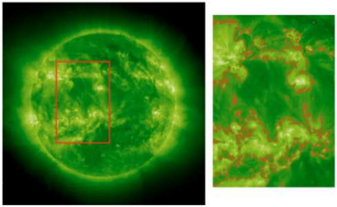
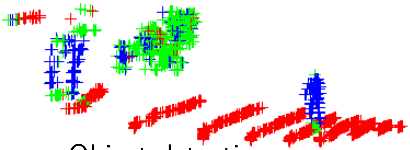




Object detection

Clustering : a technique of Machine Learning

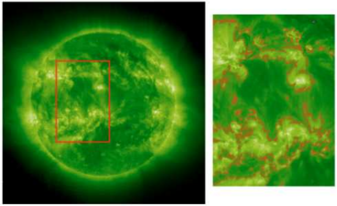
Machine

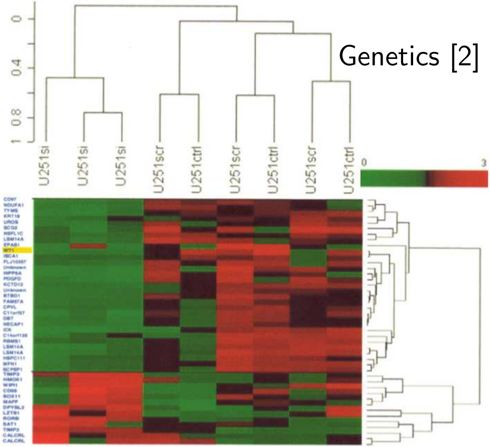
Unsupervised learning

clustering

visualization

Astronomy [1]





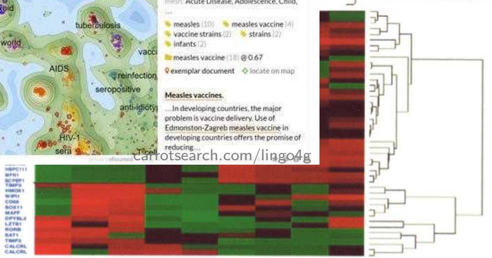
Genetics [2]

Object detection

Clustering : a technique of Machine Learning

Text mining

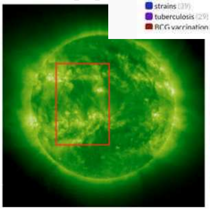
Genetics [2]

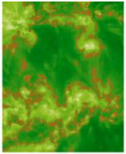


Unsuperv

clustering

Astronomy [1]

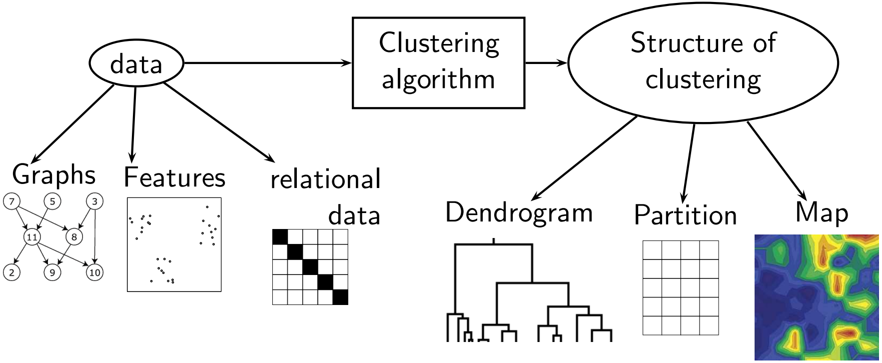




Object detection

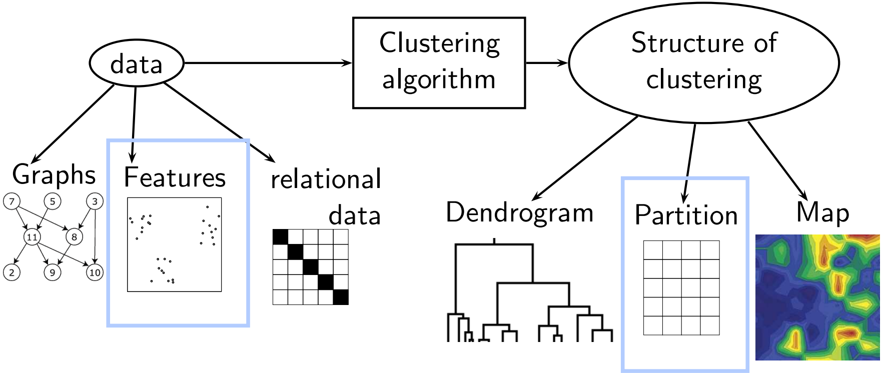
Clustering

Determine the group of objects following a similarity notion



Clustering

Determine the group of objects following a similarity notion



Partition types

- Let $\mathbf{X} = (\mathbf{x}_i)$ be a collection of objects s.t. $\mathbf{x}_i \in \mathbb{R}^p$,
- $\Omega = \{\omega_1 \dots \omega_c\}$ a set of c clusters,

Hard and soft partitions:

- hard/crisp partition
- fuzzy partition
- possibilistic partition
- rough partition
- credal partition

Outline : the soft variants of k-means

1. k-means
2. fuzzy c-means
3. rough k-means
4. possibilistic c-means
5. evidential c-means
6. Conclusion

Outline

1 k-means

2 fuzzy c-means

3 rough k-means

4 possibilistic c-means

5 evidential c-means

6 Conclusion

Hard partition

- Each object is assigned to one and only one cluster
- $\mathbf{P} = (p_{ik})$ s.t $p_{ik} \in \{0, 1\}, \sum_{k=1}^{c} p_{ik} = 1$

Example

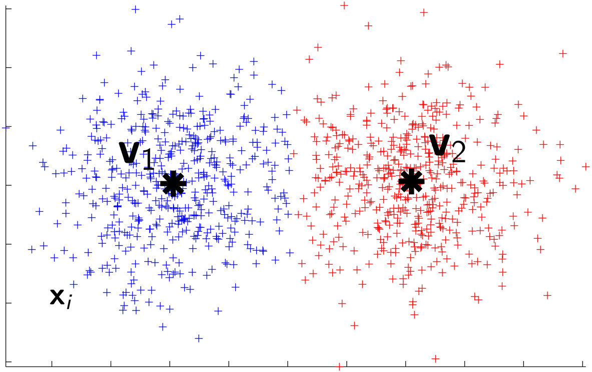
Let ω_1 be the class of square, ω_2 the class of round

	p_{i1}	p_{i2}
○	0	1
□	1	0
□	1	0

k-means

Geometrical model:

- Each cluster ω_k is represented by a center $\mathbf{v}_k$
- Euclidean distance $d_{ik}^2 = \|\mathbf{x}_i - \mathbf{v}_k\|^2$



k-means

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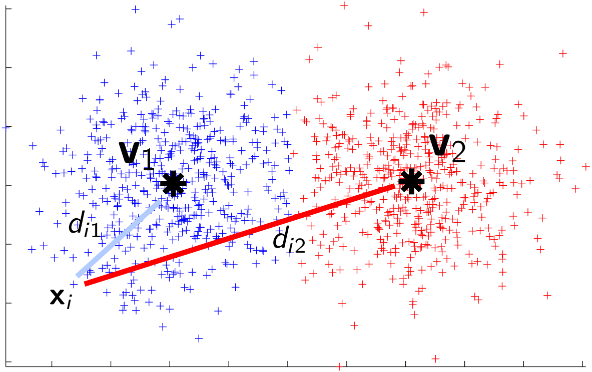


k-means

Objective function

$$J_{KM} = \sum_{i=1}^{N} \sum_{k=1}^{c} p_{ik} d_{ik}^2$$

Subject to

$$\sum_{k=1}^{c} p_{ik} = 1 \text{ and } p_{ik} \in \{0, 1\} \forall i, k$$

Optimization

NP-Hard $\Rightarrow$ minimization using an iterative procedure:

$$\text{fix } \mathbf{V}, \min_{\mathbf{P}} J_{KM} \quad \rightleftarrows \quad \text{fix } \mathbf{P}, \min_{\mathbf{V}} J_{KM}$$

Advantage

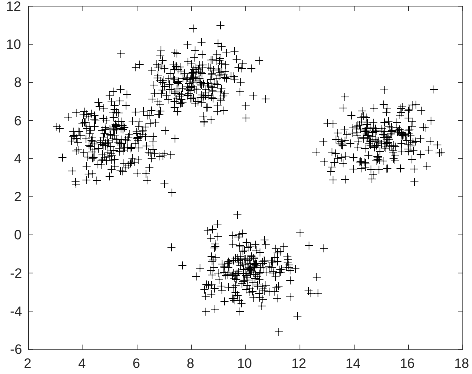
Fast

Disadvantage

Risk of local minimum

Determination of the number of clusters

GaussK4 dataset

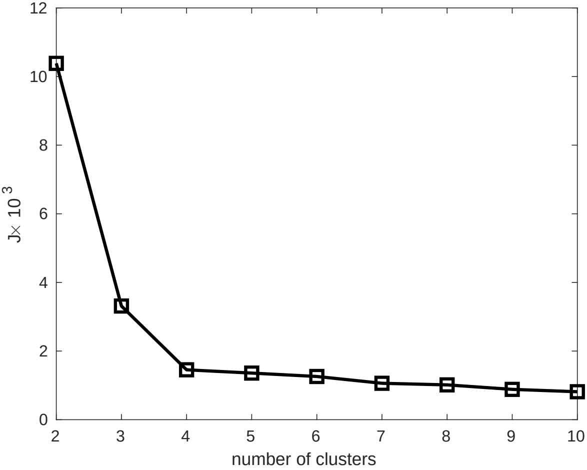


For c=1 to 10

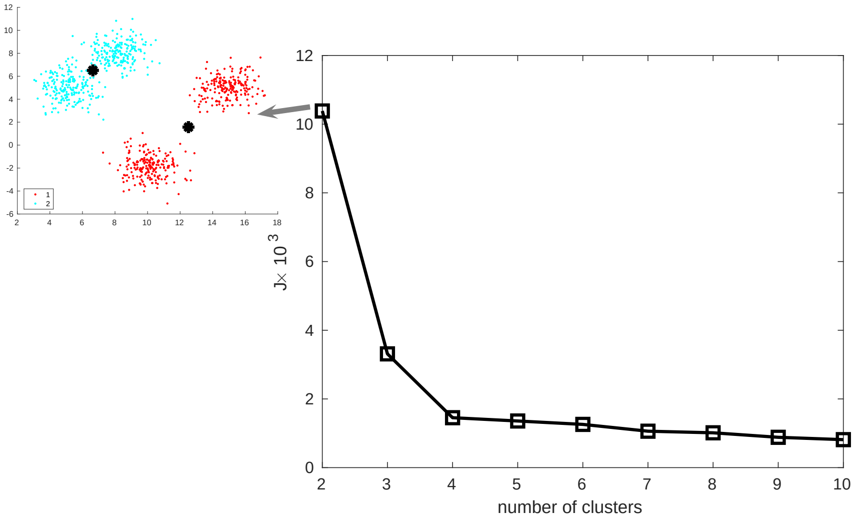
- run kmeans
- evaluate the partition

Plot evaluation measure vs number of clusters

Determination of the number of clusters



Determination of the number of clusters



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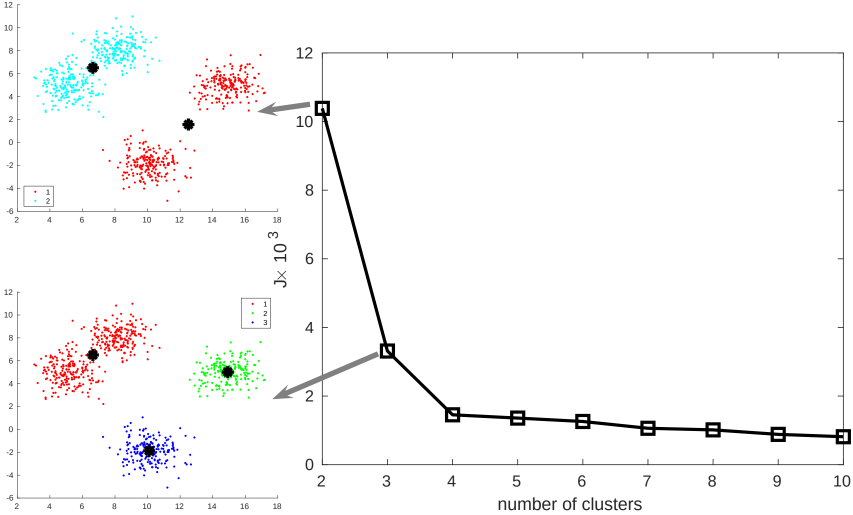
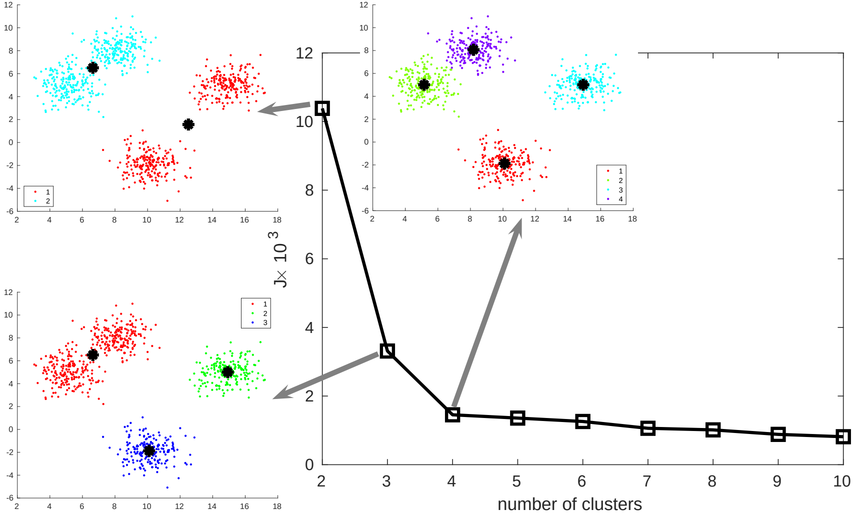


Determination of the number of clusters



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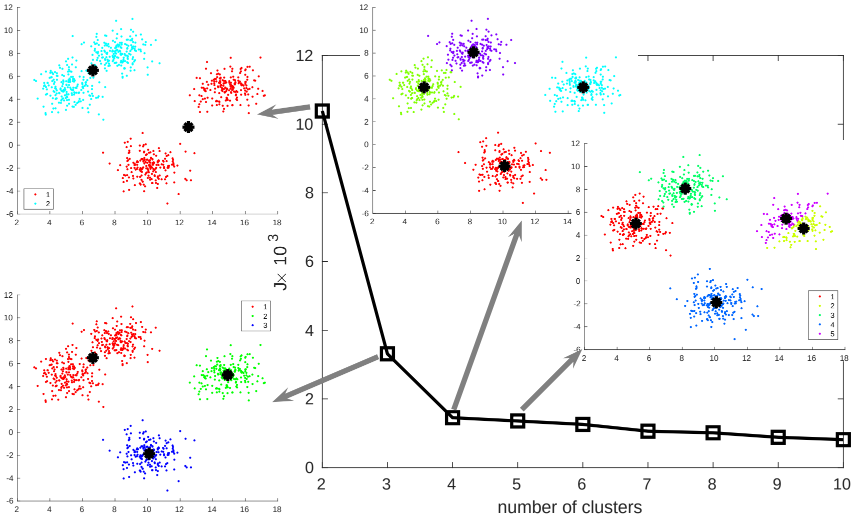

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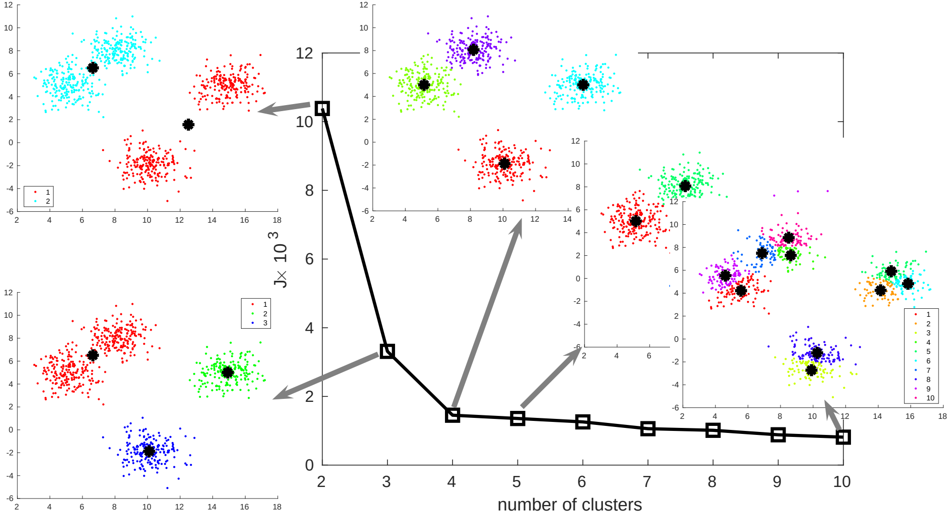
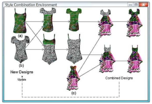
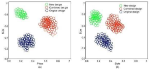
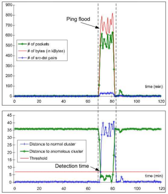


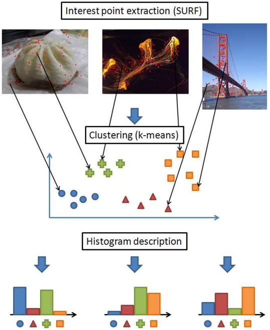
Applications

- Biology and Bioinformatics
  - Protein structure prediction
  - Gene expression
- Engineering
  - Encoding/decoding
  - Image retrieval system
  - Color image segmentation
- Business and Economics
  - Exploration of shopping orientations [10]
  - Marketing
- Faud detection [6]









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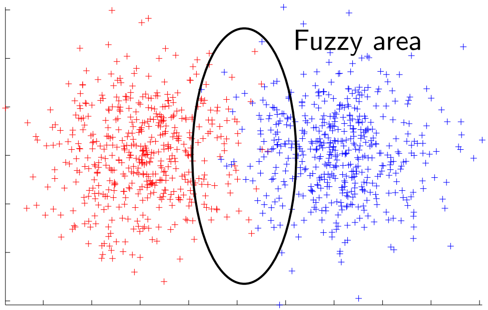
Problematic



Original data

Solution

Express uncertainty about the clustering result

Fuzzy partition

- Each object has a degree of membership to each cluster
- $\mathbf{U} = (u_{ik})$ s.t $u_{ik} \in [0, 1], \sum_{k=1}^{c} u_{ik} = 1$

Example

Let ω_1 be the class of square, ω_2 the class of round

	p_{i1}	p_{i2}
	0	1
	1	0
	0.9	0.1
	0.5	0.5

Outline

1 k-means

2 fuzzy c-means

3 rough k-means

4 possibilistic c-means

5 evidential c-means

6 Conclusion

Fuzzy c-means (FCM)

Objective function

$$J_{FCM} = \sum_{i=1}^{N} \sum_{k=1}^{C} u_{ik}^{\beta} d_{ik}^{2}$$

Subject to

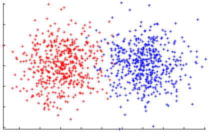
$$\sum_{k=1}^{C} u_{ik} = 1 \text{ and } u_{ik} \geq 0 \quad \forall i, k$$

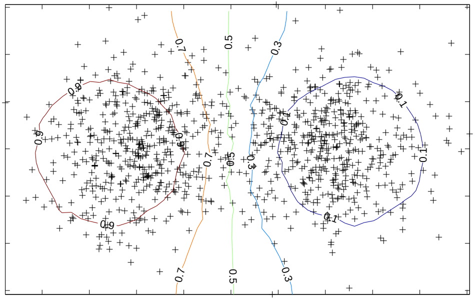
Aternate optimization

$$\min_{\mathbf{U}} J_{FCM} \quad \rightleftarrows \quad \min_{\mathbf{V}} J_{FCM}$$

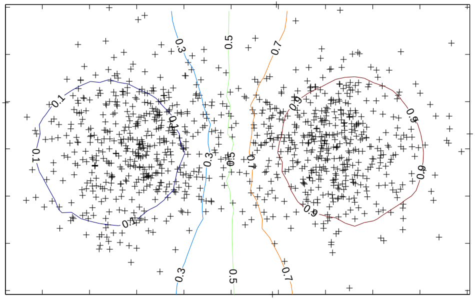
Fuzzy c-means (FCM)

Original data





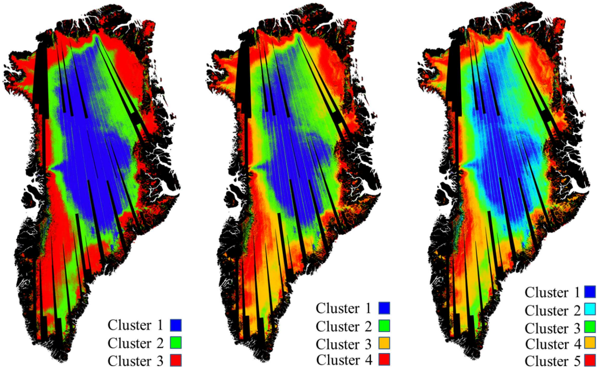
ω_1



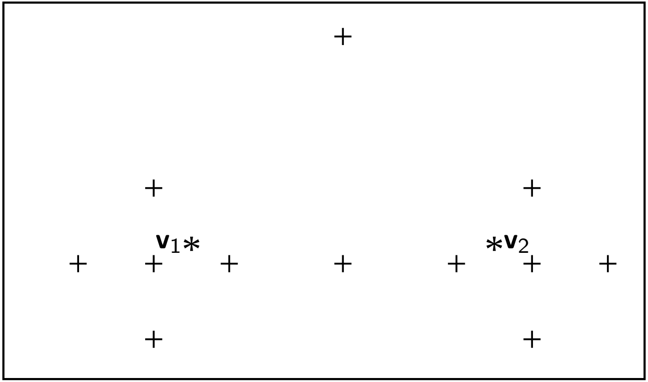
ω_2

Applications

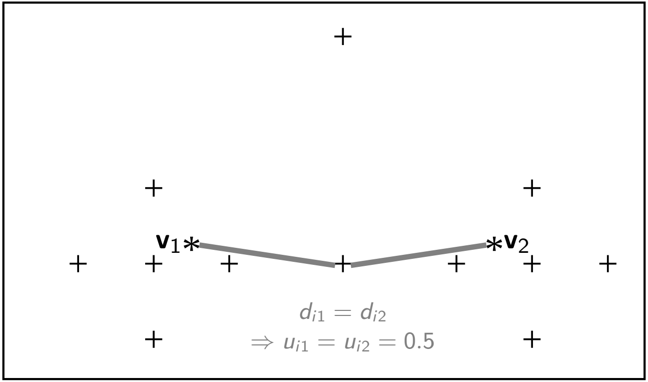
Same as k-means, but avoid decision threshold.
Example : Characterization of snow facies [8]



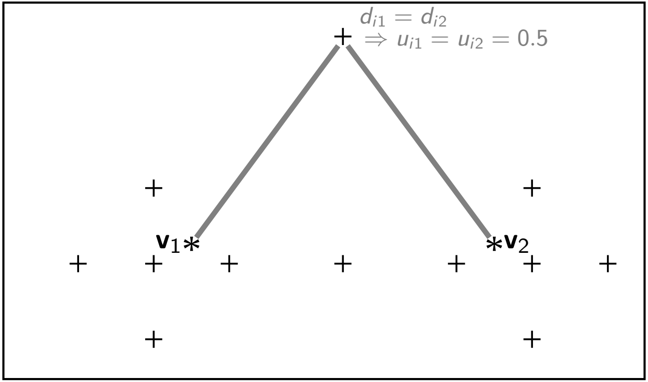
Problematic: outliers



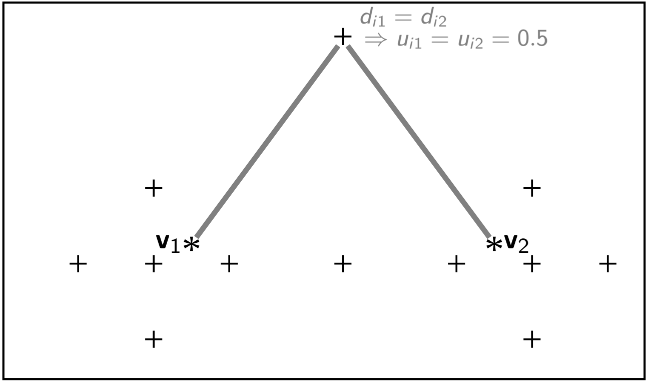
Problematic: outliers



Problematic: outliers



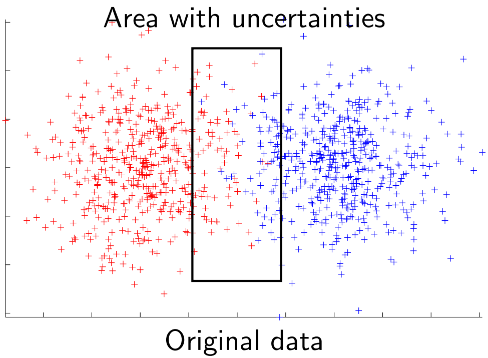
Problematic: outliers



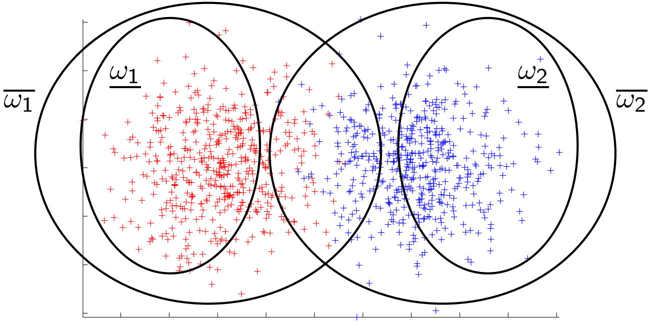
Solution

Relax the sum constraint

Problematic: where are the limits of an uncertain region ?



Problematic: where are the limits of an uncertain region ?



Original data

Solution

Express for each cluster ω_k a lower approximation $\underline{\omega}_k$ and an upper approximation $\overline{\omega}_k$

Rough partition

- Each object has a lower/upper approximation to each cluster
- $(\overline{\lambda}, \underline{\lambda}) = ((\overline{\lambda}_{ik}), (\underline{\lambda}_{ik}))$ s.t $\overline{\lambda}_{ik}, \underline{\lambda}_{ik} \in \{0, 1\}$,
  - if $\mathbf{x}_i \in \underline{\omega_k}$ then $\underline{\lambda}_{ik'} = 1$ and $\sum_{k=1}^{c} \overline{\lambda}_{ik} = 0$,
  - otherwise, $\sum_{k=1}^{c} \underline{\lambda}_{ik} = 0$ and $\sum_{k=1}^{c} \overline{\lambda}_{ik} \geq 1$.

Example

Let ω_1 be the class of square, ω_2 the class of round

	$\underline{\lambda}_{i1}$	$\overline{\lambda}_{i1}$	$\underline{\lambda}_{i2}$	$\overline{\lambda}_{i2}$
	1	0	0	0
	0	0	1	0
	0	0	1	0
	0	1	0	1

Outline

1. k-means
2. fuzzy c-means
3. rough k-means
4. possibilistic c-means
5. evidential c-means
6. Conclusion

Rough c-means

Objective function

$$J_{RCM} = \sum_{i=1}^{N} \sum_{k=1}^{C} \frac{\gamma}{\underline{n}_k} \underline{\lambda}_{ik} d_{ik}^2 + \frac{1-\gamma}{\overline{n}_k} \overline{\lambda}_{ik} d_{ik}^2$$

such that

- $\gamma \in [0\ 1]$ is a fixed weight
- $\underline{n}_k / \overline{n}_k$ are the number of objects in $\underline{\omega}_k / \overline{\omega}_k$

Subject to

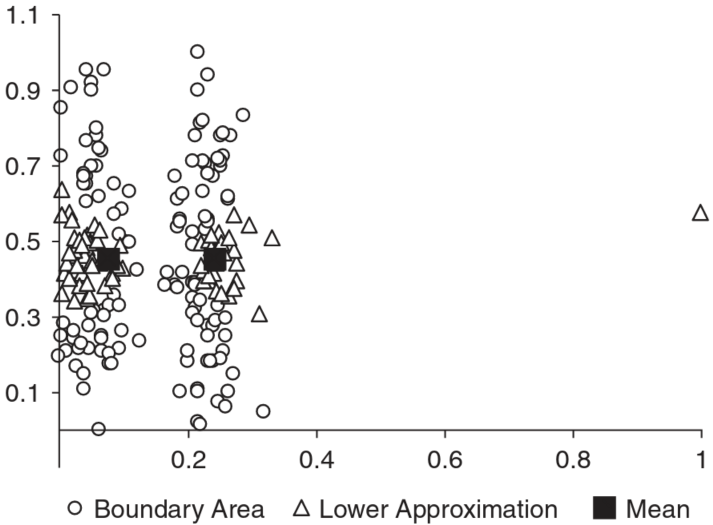
$$\left(\sum_{k=1}^{c} \underline{\lambda}_{ik} = 1 \vee \sum_{k=1}^{c} \underline{\lambda}_{ik} = 0 \right) \wedge \left(\sum_{k=1}^{c} \underline{\lambda}_{ik} = 0 \vee \sum_{k=1}^{c} \underline{\lambda}_{ik} \geq 2 \right) \text{ and}$$

$$\overline{\lambda}_{ik}, \underline{\lambda}_{ik} \in \{0, 1\} \quad \forall i, k$$

Aternate optimization

$$\min_{\underline{\lambda}, \overline{\lambda}} J_{RCM} \quad \rightleftarrows \quad \min_{\mathbf{V}} J_{FCM}$$

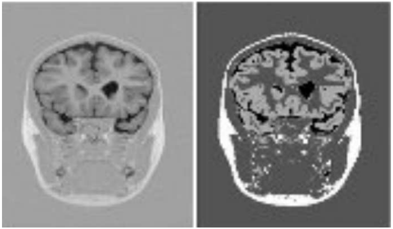
Rough c-means [7]

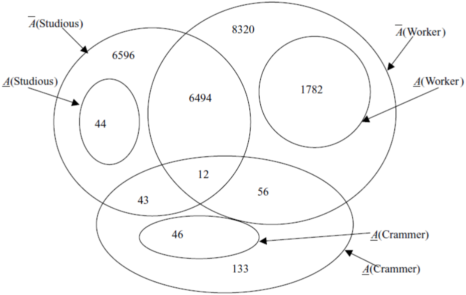


Applications

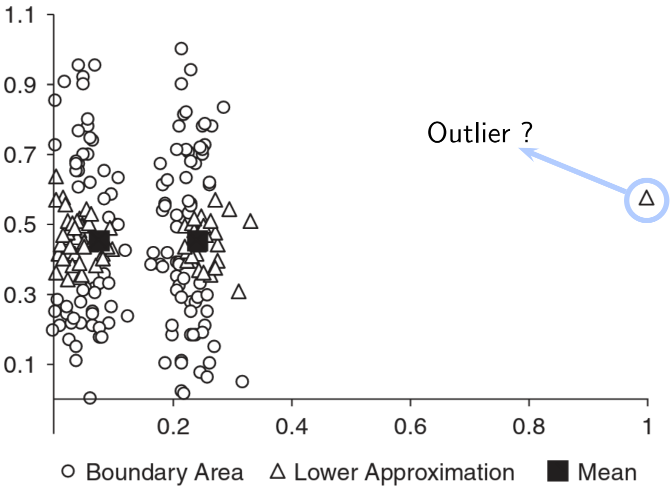
Great interest on boundary regions:

- Biology and Bioinformatics
- Medical imagery [5]
- Forest cover data
- Business and Economics
- Website profiles [4]
- ...





Problematic



Possibilistic partition

- Each object has a degree of possibility to each cluster
- $\mathbf{T} = (t_{ik})$ s.t $t_{ik} \in [0, 1]$

Example

Let ω_1 be the class of square, ω_2 the class of round

	t_{i1}	t_{i2}
	0	1
	1	0
	1	0.1
	1	1
	0	0

Possibilistic transformations

Possibilistic partition

	t_{i1}	t_{i2}
○	0	1
□	1	0
□	1	0.1
◗	1	1
☆	0	0

normalization

$$u_{ik} = \frac{t_{ik}}{\sum_{k=1}^{c} t_{ik}}$$

Fuzzy partition

	u_{i1}	u_{i2}
○	0	1
□	1	0
□	0.91	0.09
◗	0.5	0.5
☆	?	?

maximum

$$p_{ik} = \max_{k=1}^{c} t_{ik}$$

Hard partition

	p_{i1}	p_{i2}
○	0	1
□	1	0
□	1	0
◗	?	?
☆	?	?

Outline

1. k-means
2. fuzzy c-means
3. rough k-means
4. possibilistic c-means
5. evidential c-means
6. Conclusion

Possibilistic c-means (PCM)

Objective function

$$J_{PCM} = \sum_{i=1}^{N}\sum_{k=1}^{C} t_{ik}^{\beta} d_{ik}^{2} + \sum_{k=1}^{c} \gamma_k \sum_{i=1}^{N} (1 - t_{ik})^m$$

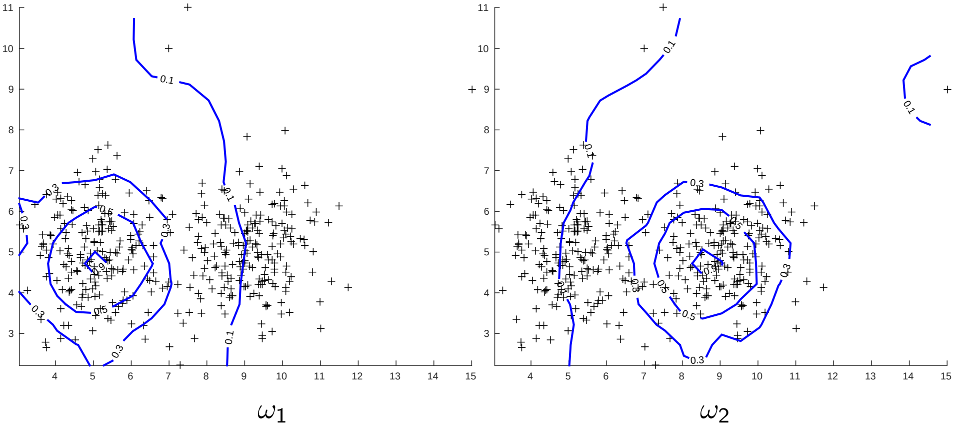
Subject to

$$t_{ik} \geq 0 \quad \forall i, k$$

Aternate optimization

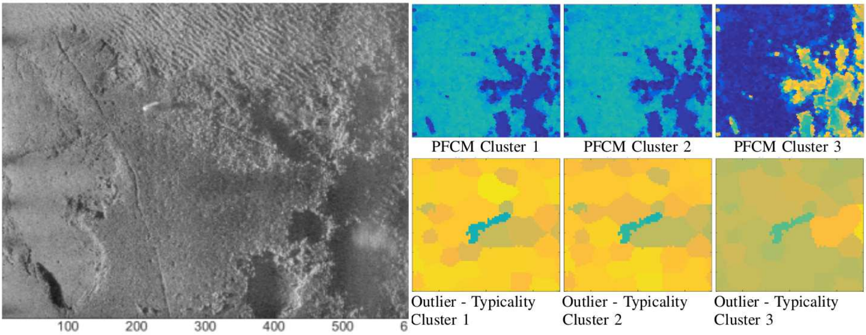
$$\min_{\mathbf{T}} J_{PCM} \quad \rightleftarrows \quad \min_{\mathbf{V}} J_{PCM}$$

Possibilistic c-means (PCM)



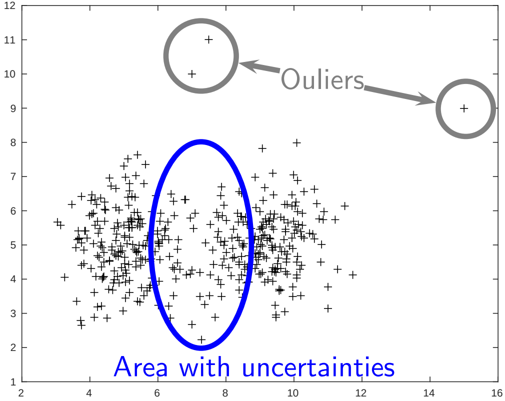
Applications

Same as FCM, but handles outliers.
Example : sonar image segmentation [11]



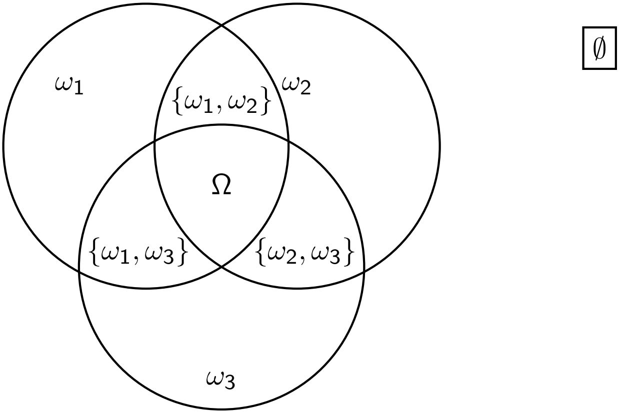
Problematic

Can we represent uncertain region and outliers with a mathematical framework ?



Credal partition

Uncertainties represented with subsets of $\Omega = \{\omega_1, \ldots, \omega_c\}$



Credal partition

- Each object has a degree of belief to each subset $A_j \subseteq \Omega$
- $\mathbf{M} = (m_{ij})$ s.t $m_{ij} \in [0, 1]$, $\sum_{A_j \subseteq \Omega} m_{ij} = 1$

Example

Let ω_1 be the class of square, ω_2 the class of round

	$m_{i\emptyset}$	$m_{i\omega_1}$	$m_{i\omega_2}$	$m_{i\Omega}$
	0	0	1	0
	0	1	0	0
	0	0.9	0.1	0
	0	0	0	1
	1	0	0	0

Derivative notions

Belief function

Total support given to A:

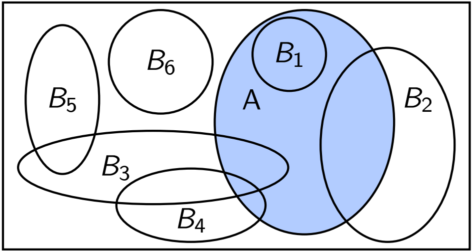
$$bel(A) = \sum_{B \subseteq A} m(B),$$

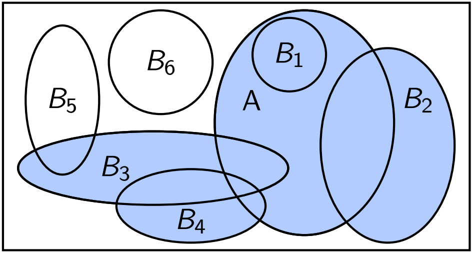
Plausibility function

Potential degree of belief that *could be* given to A:

$$pl(A) = \sum_{B \cap A \neq \emptyset} m(B),$$

$$\forall A \subseteq \Omega, A \neq \emptyset$$





Credal transformations

Credal partition

	$m_{i\emptyset}$	$m_{i\omega_1}$	$m_{i\omega_2}$	$m_{i\Omega}$
○	0	0	1	0
□	0	1	0	0
▢	0	0.9	0.1	0
D	0	0	0	1
☆	1	0	0	0

→ plausibility →

Possibilistic partition, $\rightsquigarrow \overline{\lambda}$

	t_{i1}	t_{i2}
○	0	1
□	1	0
▢	0.9	0.1
D	1	1
☆	0	0

→ belief →

$\rightsquigarrow \underline{\lambda}$

	t_{i1}	t_{i2}
○	0	1
□	1	0
▢	0.9	0.1
D	0	0
☆	0	0

Credal transformations

Making decision : the pignistic transformation

$$BetP(\omega) = \frac{1}{1 - m(\emptyset)} \sum_{\{A \subseteq \Omega | \omega \in A\}} \frac{m(A)}{|A|}$$

Credal partition

	$m_{i\emptyset}$	$m_{i\omega_1}$	$m_{i\omega_2}$	$m_{i\Omega}$
○	0	0	1	0
□	0	1	0	0
▢	0	0.9	0.1	0
D	0	0	0	1
☆	1	0	0	0

pignistic → transformation

Fuzzy partition

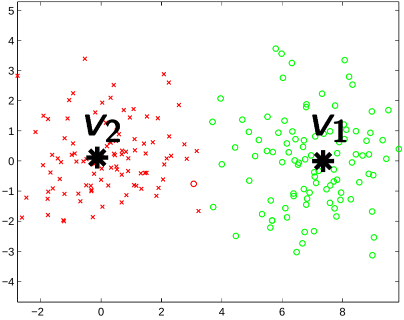
	$u_{i\omega_1}$	$u_{i\omega_2}$
○	0	1
□	1	0
▢	0.9	0.1
D	0.5	0.5
☆	0.5	0.5

Outline

1. k-means
2. fuzzy c-means
3. rough k-means
4. possibilistic c-means
5. evidential c-means
6. Conclusion

Evidential c-means (ECM)

- Each cluster ω_k is represented by a center $\mathbf{v}_k$
- Centroid $\overline{\mathbf{v}}_j$: barycenter of centers associated to classes composing $A_j \subseteq \Omega$
- Distance d_{ij}^2 between $\mathbf{x}_i$ and $\overline{\mathbf{v}}_j$



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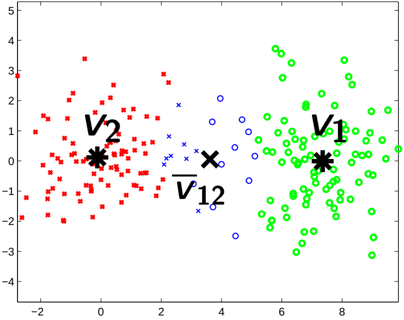


Evidential c-means (ECM)

Objective function

$$J_{ECM} = \sum_{i=1}^{N} \sum_{A_j \subseteq \Omega,\ A_j \neq \emptyset} |A_j|^\alpha m_i(A_j)^\beta d_{ij}^2 + \sum_{i=1}^{N} \delta^2 m_i(\emptyset)^\beta$$

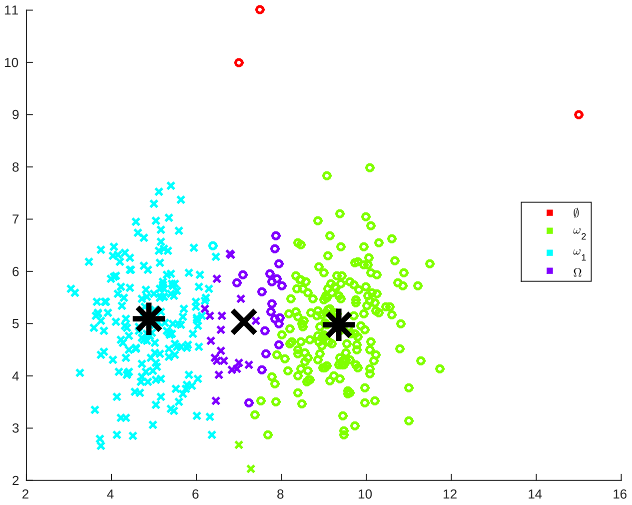
Subject to

$$\sum_{A_j \subseteq \Omega,\ A_j \neq \emptyset} m_i(A_j) + m_i(\emptyset) = 1 \text{ and } m_i(A_j) \geq 0 \quad \forall i, j$$

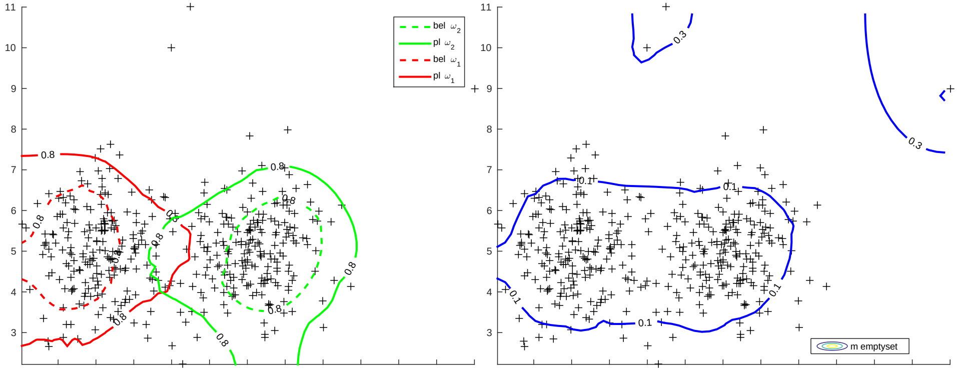
Alternate optimization

$$\text{opt}(\mathbf{M}) \leftrightarrows \text{opt}(\mathbf{V})$$

ECM: hard credal partition

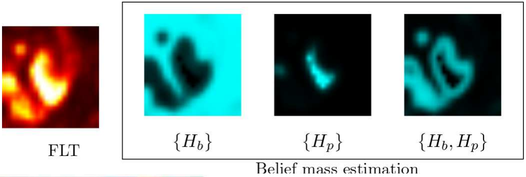


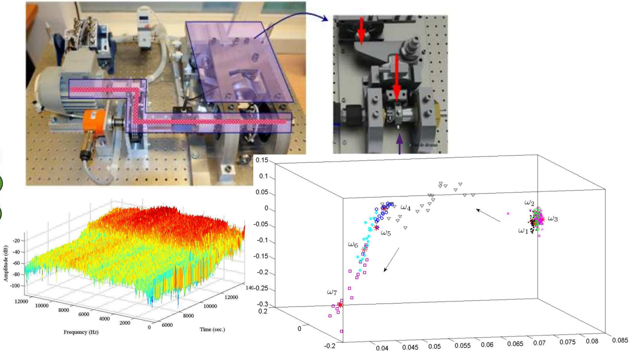
ECM: lower, upper bound and outliers

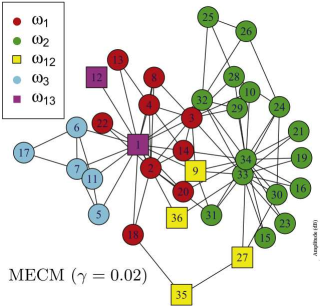


Applications

- medical image processing [3]
- machine prognosis [9]
- analysis of social networks [12]

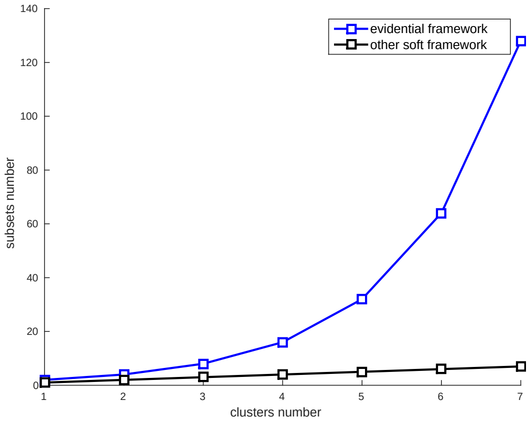






Problematic

c clusters $\Rightarrow 2^c$ subsets !



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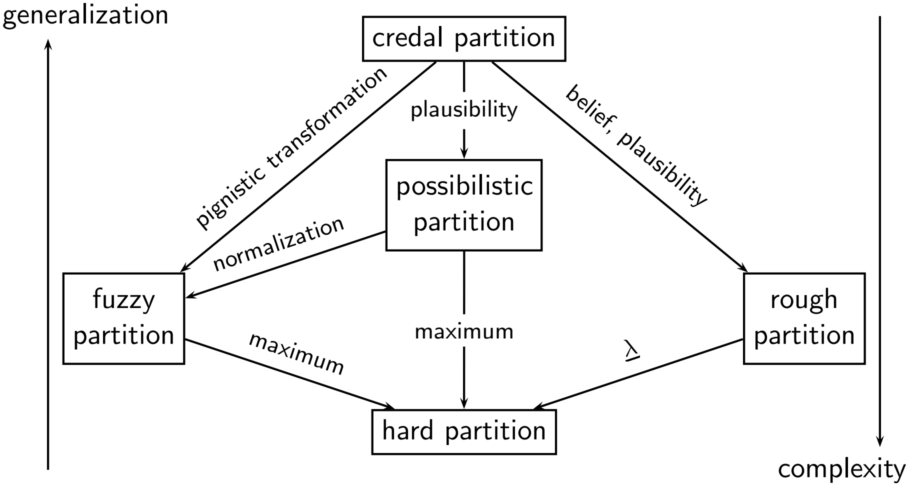
Clustering

- *k-means*
  - \+ real time constraint, big data, hard decision to make
- *fuzzy c-means*
  - \+ handle overlapped clusters
- *rough k-means*
  - \+ hard decision to make with overlapped clusters, upper and lower belief on that decision
- *possibilistic c-means*
  - \+ separate analysis of each cluster results, outliers
  - \- mathematical framework with properties complex to handle
- *evidential c-means*
  - \+ strong partition analysis possible
  - \- small number of clusters

Partition types



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Thank you