

Fuzzy and Evidential Contribution to Multilevel Clustering

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Keywords: Multilevel Clustering, Cmeans, Ecm, Split Criterion, Fuzzy Silhouette, Credal Partition, Spectral Clustering.

Abstract: Clustering algorithms based on split-and-merge concept, divisive or agglomerative process are widely developed to extract patterns with different shapes, sizes and densities. Here a multilevel approach is considered in order to characterise general patterns up to finer shapes. This paper focus on the contribution of both fuzzy and evidential models to build a relevant divisive clustering. Algorithms and both *a priori* and *a posteriori* split criteria are discussed and evaluated. Basic crisp/fuzzy/evidential algorithms are compared to cluster four datasets within a multilevel approach. Finally, same framework is also applied in embedded spectral space in order to give an overall comparison.

1 INTRODUCTION

Extracting general behaviours or particular patterns in data is a common task in various industrial, medical or environmental applications. K-means and its derivative algorithms are appreciated for their understandability and explicability of the resulting clusters. They also are low-cost algorithms on several aspects including computation time, development time, energy. However, in real-life datasets, clusters can have different sizes, densities, shapes (non-convex, related or thread-like) and ambiguous boundaries. Algorithms such as K-means don't perform well on such diverse datasets, but other clustering approaches such as spectral or multilevel ones suit more. In the past decades, several multilevel methods were developed in order to work at different scales depending on the cluster's shape.

To deal with non-linearly separable clusters, spectral approaches were proposed, with the aim to transfer data into an embedded spectral space, where the boundaries between clusters become linear. Numerous clustering problems are based on multiscale problems, leading to the emergence of multilevel clustering such as recursive biparted spectral clustering algorithm (Shi and Malik, 2000), spectral hierarchical clustering HSC (Sanchez-Garcia et al., 2014) or MSC (Grassi et al., 2019). But computing spectral embedded spaces is time-consuming when applied on normal/large datasets and can result in not perfectly accu-

rate clustering results when noise and ambiguity appears.

Fuzzy/evidential partition could help to deal with such noisy datasets. We propose to compare a large diversity of clustering approaches, on a selection of possibly noisy datasets: crisp vs fuzzy or evidential, direct vs multilevel/hierarchical, working in the raw initial features space or in a spectral embedded space.


This paper is organised as follows: Section 2 provides multilevel clustering background and a presentation of their split criteria. Section 3 gives the general protocol of the methods evaluation and Section 4 analyses the results to highlight benefits and drawbacks of each method.

2 MULTILEVEL CLUSTERING, CONCEPT AND PARAMETERS

2.1 Multilevel Approach

A divisive hierarchical clustering approach is used to build a multilevel structuring of datasets: from global shapes to finer parts leading to a more precise analysis of datasets. An illustration of a three-level clustering is given by Figure 1 (Grassi et al., 2019).

This process can be carried out either from the features data or from an embedded space. In both cases, data would may be first normalised if necessary (min-max scaling for instance).

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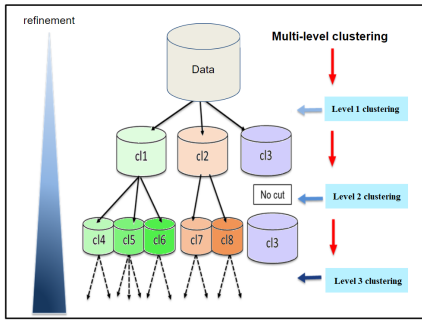


Figure 1: Multilevel clustering approach.

2.1.1 Multilevel Clustering Framework

Algorithm 1 describes the general MultiLevel Clustering framework (MLC). At each level, for each clustering, the number of clusters K is *a posteriori* selected by maximising the silhouette criterion of the K-means algorithm. Then, the sub-dataset is clustered into K clusters. For each cluster, a split criterion is computed to assess its quality/compactness (cf. Section 2.2). If the criterion doesn't reach a given threshold, the algorithm restarts the same clustering procedure on it. The whole process stops either when the maximum level is reached, or when all clusters verify the split-criterion's threshold.

Algorithm 1: Multilevel clustering framework.

```

Require:  $X$  data,  $-1 \leq chosenThreshold \leq 1$ 
Require:  $MaxLevel \geq 1, MaxK \geq 1$ 
 $clToSplit \leftarrow \{1\}; NextclToSplit \leftarrow \{\}$ 
 $treeLabelled \leftarrow NULL$ 
 $level \leftarrow 1$ 
while  $clToSplit \neq \{\}$  and  $level \leq levelMax$  do
  for  $X \in clToSplit$  do
     $K_X \leftarrow \arg \max_{k \in [2, maxK]} silhouette(clustering(X, k))$ 
     $clust_X \leftarrow clustering(X, K_X)$ 
     $treeLabelled \leftarrow appendTree(clust_X)$ 
    for  $Y \in clust_X$  do
       $criteriaCluster \leftarrow ComputeSplitCriterion$ 
      if  $criteriaCluster \leq chosenThreshold$  then
         $NextclToSplit \leftarrow Y \cup NextclToSplit$ 
      end if
    end for
  end for
   $level \leftarrow level + 1$ 
   $clToSplit \leftarrow NextclToSplit; NextclToSplit \leftarrow \{\}$ 
end while
return  $treeLabelled$ 

```

2.1.2 Embedded Space Variant

To relax data shape requirements and to avoid the selection of one suitable partitioning algorithm, each clustering may be applied in the embedded space

generated by Algorithm 2 (# means cardinal number). This space consists in the K first eigenvectors of the NJW Laplacian L (Ng and Weiss, 2001), built from the local kernel gaussian ZP-similarity matrix W (Zelnik-manor and Perona, 2004). At each level, K is set to the number of the largest Principal EigenValues PEV of L .

Algorithm 2: Spectral clustering with K estimation.

```

Require:  $X, neighbour, PEVthreshold$ 
 $W \leftarrow ZP.similarity.matrix(X, neighbour)$ 
 $W \leftarrow check.gram.similarityMatrix(W)$ 
 $L \leftarrow compute.laplacian.NJW(W)$ 
 $K \leftarrow \#(W\$eigenValues > PEVthreshold)$ 
 $dataSpec \leftarrow W\$eigenVectors[, 1 : K]$ 
 $clust_X \leftarrow clustering(dataSpec, K)$ 
return  $clust_X$ 

```

2.2 Stopping Split Criteria

In multilevel clustering, split criterion is an important feature. This criterion can direct the clustering towards geometry-based clustering, density-based clustering, etc.

The first 3 split criteria studied are *a priori* criteria: they estimate the necessity of a subdivision (without doing it). They assess the homogeneity of the clusters: low values indicate that they should be subdivided. They are:

- The number of wrongly-clustered points named $CardSil$, with $CardSil = \#(silhouette_i < 0) < CardThreshold, i \in cluster C_k$, as implemented in the R-package *sClust*. A threshold set to 0 requires that all points are closer to its cluster's neighbours than to points of other clusters.
- The average silhouette of a cluster named $Sil = mean(silhouette_i) > SilThreshold, i \in [1; C_k]$. It evaluates the overall geometry of a given cluster. By heuristics, $SilThreshold$ is set to 0.7.
- A fuzzy generalisation of the silhouette criterion: the Fuzzy Silhouette (Campello and Hruschka, 2006). This fuzzy silhouette (FS) can be interpreted as the silhouette criterion of the cluster cores: it decreases the impact of ambiguous points.

All the above criteria are *a priori* split criteria. If the value of the criterion doesn't reach a certain threshold, the clustering of the sub-dataset is computed. We also propose an *a posteriori* criterion to deal with fuzzy and evidential approaches:

- The *Mass* criterion is based on fuzzy or evidential membership functions. This criterion evalu-

ates the quality of a level clustering by assessing the non-ambiguity between clusters:

$$Mass = \frac{1}{K} \sum_{k=1}^K \frac{1}{\#C_k} \sum_{i \in C_k} m_i(C_k)$$

Indeed, for each point i of the obtained defuzzified cluster C_k , $m_i(C_k)$ denotes the membership degree of i to C_k : the higher the value, the lower the ambiguity of its cluster assignment. So, a high *Mass* value means that the obtained current clustering is coherent: it should be kept, and a sub-clustering level may then be considered. Conversely, a low value means that the obtained clustering should not be kept, because of its high ambiguity. In section 4, 2 variants of this criterion are going to be compared *Mass25* and *Mass100*: *Mass100* denotes the original *Mass* criterion, whereas *Mass25* is a more selective variant which averages the 25% lowest membership degrees of each cluster.

3 COMPARISON PROTOCOL

In order to compare approaches, a protocol has been set up. Considering the variety of algorithms, several protocols are explained in this section. Furthermore, parameters settings is also described. Then, quality criteria are listed followed by there explanation. Finally, datasets are shown.

3.1 Clustering Algorithms Compared

In order to evaluate fuzzy and evidential contribution to multilevel clustering, 3 types of algorithms are compared:

- **Direct Algorithms** such as K-means, *cmeans* (*e1071* :: *cmeans*) as fuzzy algorithm and *ecm* (*evclust* :: *ecm*) algorithm (Masson and Dencœux, 2007) for credal clustering as witness values.
- **Agglomerative Algorithms** such as high-density based scanning (*dbscan* :: *hdbscan*), agglomerative Ward.d2 clustering (*stats* :: *hclust*) and HSC (*sClust* :: *HierarchicalSC*) to compare how well the fuzzy and evidential multilevel algorithms perform well on dense datasets.
- **Multilevel Algorithms** based on the previous direct algorithms in the initial and spectral clustering space.

3.2 Overview of the General Protocol

During the process, it is necessary to ensure a good convergence of all elementary clustering. Thus, each

clustering is computed 10 times, and the best result is kept, according to its own optimization's criteria.

Moreover, global clustering approaches are iterated 10 times to make the assessment more robust. The mean value of each quality criterion is computed as the final result (standard deviation near zero, not shown).

3.3 Parameter Settings

Let K^* be the ground truth number of classes. For direct approach and agglomerative clustering based on Ward, the K input is set to K^* . For others methods, K is estimated in order to be close to the ground truth.

3.3.1 K Estimation: A "Fair" Estimation Method

At each level of multilevel approaches, a number of clusters K has to be automatically determined. Two methods are used, depending on the working space used.

In the initial space, K is determined using silhouette criterion. Silhouette criterion is computed for each $i \in \llbracket 2, 10 \rrbracket$ and the i value maximizing the silhouette criteria is chosen as the optimal K value.

In spectral embedded space, K is set as the number of prime eigenvalues of Laplacian matrix, which are higher than a *PEVthreshold* (0.999 by default, i.e. close to 1-value for numerical error computation)

3.3.2 Split Threshold Estimation: A Supervised Method

Split threshold has a huge impact in multilevel approaches that could stop clustering to its first level or result in an over-clustering. In order to avoid an *a priori* threshold leading to this kind of aberrant final number of clusters, it is rather computed following Algorithm 3. The threshold is iteratively tuned, either by incrementation or decrementation depending on the split criterion, until the number of clusters reaches the true number of classes.

3.4 Agglomerative Algorithms: A Specific Evaluation Protocol

Two agglomerative methods compared in this paper have specific architectures, which require specific parameter settings.

- **HC -Ward D2 clustering** (*stats::hclust*) builds a clustering tree according to within-cluster variance minimum. Then, dendrogram is cut (*stats::cutree*) according to a K^* value.

- **dbscan::hdbscan** agglomerates points according to a core density with a minimum number of points per cluster (*minPts*). Two different values of *minPts* parameter are considered to reach the K^* ground truth: the closest lower and upper K value.

Algorithm 3: Threshold determination.

Require: *data*, *SplitCriterion*, K^*
if *SplitCriterion* == *mass* **then**
 threshold \leftarrow 1
else
 threshold \leftarrow -1
end if
NbFinalCluster \leftarrow 0
while *NbFinalCluster* < K^* **do**
 if *SplitCriterion* == *mass* **then**
 threshold \leftarrow *threshold* - 0.05
 else
 threshold \leftarrow *threshold* + 0.05
 end if
 cluster \leftarrow *MLclustering*(*data*, *threshold*)
 NbFinalCluster \leftarrow #*unique*(*cluster*)
end while
return *threshold*

3.5 Quality Criteria

To evaluate and compare clustering algorithms, several unsupervised quality criteria are computed:

- **The Silhouette Score**, *cluster* :: *silhouette* (Mächler et al., 2012) measures compactness of a cluster compared to the minimum inter-cluster distance. A silhouette score of 1 means that each clusters is compact and distant whereas a negative score means that inter-cluster distance are smaller than intra-cluster distance.
- **The Adjusted Rand Index**, *pdfCluster* :: *adj.rand.index* (Azzalini and Menardi, 2013) is a corrected-for-chance Rand Index. It measures the ratio of the agreement between the true and the predicted partitions over the total number of pairs.
- **The non-Overlap**, corresponds to a part of the Rand Index. The non-overlap index measures the ratio of non-overlapping pairs over the total number of pairs. A value of 1 means that all points are affected to non-overlapping clusters (a cluster included in a class) and that real classes could be retrieved.

After assigning clusters to classes using majority vote, two adapted supervised quality criteria are added to catch non representation of one ground truth

class in the obtained clusters and to detect small shapes:

- **Precision***: $\frac{1}{K^*} \times \sum_{i \in [1, K^*]} \alpha_i \times \frac{TP_i}{(TP_i + FP_i)}$
- **Recall***: $\frac{1}{K^*} \times \sum_{i \in [1, K^*]} \alpha_i \times \frac{TP_i}{(TP_i + FN_i)}$

With K^* the number of classes, the numbers *TP*: True positive, *FP*: False Positive, *FN*: False Negative and $\alpha_i = 1$ if no cluster is assigned in class i , 0 otherwise. Sometimes, majority vote doesn't perform well and small classes are affected to bigger ones. So α term penalises non represented classes in the standard precision and recall formula.

3.6 Data Presentation

Considering the diversity of clustering algorithms, different types of datasets are compared based on their specificity. Some datasets favour some algorithms (e.g. hierarchical algorithms are designed for dense datasets, fuzzy and evidential algorithms are made to characterise ambiguity...). Thus, 3 types of datasets are used in this comparison: two are non ambiguous and dense datasets, and the last one has ambiguity and uncertainty. A representation of the 3 datasets can be seen figure 2.

- **(A) Aggregation (Gionis et al., 2007)** is a well-segmented dataset composed of 7 clusters. In this seven clusters, two pairs of clusters are connected by few points, which usually disturbs the classical hierarchical clustering, such as HDBSCAN (McInnes et al., 2017) or *stats::hclust*.
- **(B) Coumpound (Zahn, 1971)** is a 2-level dataset composed of 3 clusters that can be divided into 2 clusters. A pair of clusters has the same specificity as aggregation dataset (they are connected by few points). Another pair of clusters is made in a way that one is included into the other. These two clusters are merged in order to not penalise some clustering algorithms in raw feature space; they can be easily separated using spectral approaches. The last pair is a cluster surrounded by a noise cluster.
- **(C) 6-Bananas** is a dataset built using the function *evclust::bananas* (Deneux, 2021). This dataset is designed for multilevel approaches. Three sets of bananas are positioned the same way as Coumpound dataset. This dataset is made for fuzzy and evidential clustering according to its non-linear cut between bananas.

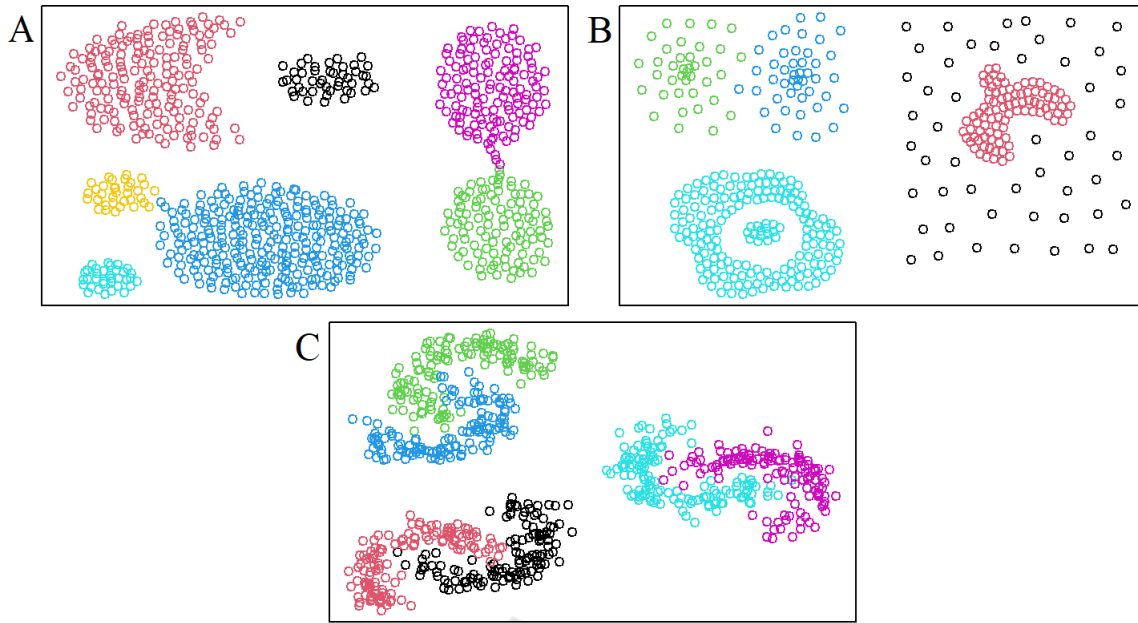


Figure 2: Datasets used with ground truth classes, one color per class - (A) Aggregation - (B) Compound - (C) 6-Bananas.

4 RESULTS AND ANALYSIS

In order to understand how well fuzzy and evidential algorithm perform, the analysis will begin with datasets where current multilevel approaches perform well. Finally, a focus on Bananas dataset will be presented where fuzzy and evidential methods are more appropriate.

4.1 Aggregation and Compound Dataset Results

Aggregation and Compound are first clustered in spectral embedded space (cf. the upper part of Table 1). The main quality criterion analysed is ARI, well-suited to the unsupervised approach.

Compound results of multilevel C-means (Mass25/Mass100) as well as multilevel K-means (CardSil) have high ARI scores. A deeper understanding of these values is given in the following rows. *Precision** and *Recall** scores show that multilevel K-means isn't as efficient as multilevel C-means. Those lower scores can be primarily explained by a class disappearance induced by a lower number of resulting clusters.

This low number of final clusters obtained by the ML K-mean (CardSil) algorithm (cf. fifth row of Table 1), can't be increased because of the architecture of the split criterion. Indeed, the roughest threshold value is already selected. This highlights a limit

of this split criterion: it may stop sub-clustering too early, if a cluster appears "coherent", despite being composed of several subclusters.

Aggregation results show that multilevel ECM (Mass25) perfectly retrieves real classes: its ARI score almost reaches 1. Multilevel K-means (Sil), C-means (FS/Mass25/Mass100) and ECM (FS/Mass100) have a high precision value but over-cluster the dataset. However, it should be noted that Mass split-criteria can lead to lower number of clusters than FS/Sil criteria.

In order to challenge a bit more algorithms, clustering is also performed in the initial features space. According to ARI, Aggregation is the most difficult dataset for fuzzy and evidential methods. Hierarchical clustering performs well on this dataset; and multilevel K-means is the best multilevel algorithm with only few overlapping pairs (less than 2%) and a good precision. Compound conclusions are slightly different. Multilevel K-means (Sil) results are equal to C-means (FS) with good precision and non-overlap values but result in a total of 23 clusters whereas multilevel C-means (Mass100) and ECM (Mass100) have better ARI and non-Overlapping scores with half final clusters: on this dataset, the resulting clustering is better using fuzzy and evidential approaches.

To sum up, spectral clustering is improved on certain datasets using fuzzy/evidential clustering and is equal on others. The reason is that compact, dense and distant clusters will still remain in spectral embedded space. But if ambiguity is kept or cre-

Table 1: Clustering results obtained in embedded spectral space (top section) and raw feature space (bottom section) by: K-means (KM), C-means (CM), Evidential C-means (ECM), agglomerative Ward.d2 clustering (HC), High Density Based Scanning (HDBSCAN) with K estimation (lower and upper closest values of K) and all Multilevel variants (ML).

	Direct (1)			Agglomerative (2)		ML KM (3)		ML CM (4)			ML ECM (5)			
	KM	CM	ECM	HC	HDBSCAN	CardSil	Sil	FS	Mass25	Mass100	FS	Mass25	Mass100	
Embedded spectral space	Compound K*=6													
	ARI	0.49	0.43	0.43	0.51	0.86-0.45	0.81	0.36	0.26	0.85	0.85	0.26	0.58	0.58
	NonOverlap	0.92	0.91	0.91	0.92	0.94	0.92	1	1	0.94	0.94	1	0.99	0.94
	Precision*	0.7	0.52	0.52	0.7	0.92	0.7	0.99	1	0.94	0.94	0.99	0.97	0.94
	Recall*	0.67	0.5	0.5	0.67	0.79-0.78	0.67	0.99	1	0.83	0.83	0.99	0.93	0.83
	NbClusters	6*	6*	6*	6*	5-7	4	17	28	7	7	21	14	13
	Aggregation K*=7													
	ARI	0.96	0.95	0.77	0.99	0.99-0.44	0.81	0.33	0.29	0.85	0.29	0.29	0.96	0.45
	NonOverlap	1	1	0.99	1	1-0.97	0.93	1	1	0.97	1	1	1	1
	Precision*	0.96	0.94	0.77	0.99	0.99-0.96	0.64	0.95	1	0.84	1	1	1	1
	Recall*	0.99	0.98	0.85	0.99	1-0.89	0.71	0.99	0.99	0.85	0.99	0.99	0.99	0.99
	NbClusters	7*	7*	7*	7*	7-20	5	21	38	14	37	38	8	26
	6-Bananas K*=6													
	ARI	0.65	0.63	0.64	0.66	0.59-0.57	0.57	0.35	0.32	0.55	0.49	0.32	0.41	0.49
	NonOverlap	0.95	0.95	0.95	0.95	0.93-0.93	0.83	0.99	0.99	0.88	0.93	0.99	0.98	0.93
Precision*	0.82	0.81	0.82	0.84	0.63-0.63	0.25	0.92	0.93	0.46	0.68	0.92	0.87	0.67	
Recall*	0.82	0.81	0.82	0.83	0.72-0.71	0.5	0.91	0.92	0.61	0.74	0.91	0.85	0.74	
NbClusters	6*	6*	6*	6*	6-8	3	23	24	7	13	24	18	13	
Feature space	Compound with class fusion K*=5													
	ARI	0.57	0.51	0.48	0.59	0.76-0.84	0.5	0.28	0.28	0.45	0.8	0.35	0.47	0.83
	NonOverlap	0.94	0.95	0.93	0.94	0.94-0.98	0.74	0.94	0.94	0.79	0.97	0.94	0.79	0.94
	Precision*	0.84	0.64	0.63	0.91	0.89-0.94	0.47	0.93	0.93	0.49	0.67	0.92	0.44	0.92
	Recall*	0.74	0.6	0.59	0.79	0.76-0.9	0.4	0.8	0.8	0.5	0.7	0.8	0.48	0.8
	NbClusters	5*	5*	5*	5*	6-9	2	23	24	6	7	12	6	11
	Aggregation K*=7													
	ARI	0.76	0.74	0.55	0.81	0.81-0.67	0.66	0.56	0.52	0.63	0.59	0.55	0.52	0.52
	NonOverlap	0.99	0.99	0.92	1	0.93-0.93	0.98	0.99	0.97	0.93	0.94	0.97	0.95	0.95
	Precision*	0.76	0.76	0.47	0.79	0.64-0.64	0.95	0.97	0.79	0.65	0.66	0.76	0.67	0.67
	Recall*	0.83	0.83	0.54	0.86	0.71-0.71	0.89	0.93	0.83	0.61	0.7	0.82	0.66	0.66
	NbClusters	7*	7*	7*	7*	5-55	14	18	15	13	17	25	14	14
	6-Bananas K*=6													
	ARI	0.57	0.59	0.57	0.67	0.57-0.03	0.57	0.37	0.37	0.54	0.54	0.38	0.49	0.51
	NonOverlap	0.94	0.94	0.93	0.94	0.83-0.98	0.83	0.94	0.94	0.96	0.96	0.94	0.96	0.92
Precision*	0.76	0.78	0.79	0.86	0.25-0.92	0.25	0.93	0.73	0.84	0.84	0.72	0.8	0.63	
Recall*	0.76	0.78	0.75	0.82	0.5-0.87	0.5	0.81	0.81	0.84	0.84	0.8	0.79	0.72	
NbClusters	6*	6*	6*	6*	3-218	3	75	64	10	10	50	14	14	

ated while transferring data into spectral embedded space, fuzzy/evidential methods will improve clustering thanks to their membership characterisation.

Also, CardSil split criterion shows its limits in raw features space, because the lowest possible estimated K is often lower than the ground-truth value. Thus, finer shapes can't be retrieved, restraining multilevel approach.

4.2 A More Difficult Dataset: 6-Bananas

Bananas dataset combines several difficulties: cluster boundaries are non-linear, very close to each other, ambiguous, and the cluster densities are weak (each banana has 125 points, ambiguity included). Therefore, clustering is particularly hard.

Clustering in Spectral Space. The too high connectivity between bananas does not allow building a relevant spectral space. But this spectral space causes in most cases lower final number of clusters and homogeneous clusters (non-overlap scores are almost equal to 1).

Clustering in Raw Features Space. Direct methods with true value of K achieve quite good ARI results. However, they do not clearly exceed 0.57, the ARI score obtained by the 2 methods resulting in $K = 3$ clusters (pairs of bananas are identified, but without a finer division). HC with the true value of K gives the best clustering with an ARI equal to 0.67 and only 6% of overlapping pairs of points. HDBSCAN is not particularly efficient on this dataset. With 3 minimum points per cluster ($minPts = 3$), the algorithm gives only 3 final clusters, and when the minimum number of points per cluster is decreased to 2 points,

the algorithm gives a total of 218 clusters resulting in a disastrous ARI.

Multilevel K-means (CardSil), as mentioned above, stops at the first level and only detects the pairs of bananas.

Then two groups can be identified:

- the *Sil/FS* split criterion, which builds more than 50 final clusters. This overclustering leads to weak ARI scores. The crisp multilevel FS K-means is the worst, with 25 more clusters than ECM but the same quality criterion values.
- the *Mass25* and *Mass100* group determines between 10 and 14 final clusters. These split criteria have higher ARI (0.54 with MC CM) and almost equal non-overlap scores with less clusters, meaning that they perform better than the *Sil/FS* ones.

To summarise, fuzzy and evidential approach can improve multilevel clustering results, in spite of noisy non-linearly separable clusters. However, on this dataset, ML variants do not achieve the best ARI (HC's score), which can be explained by their higher number of final clusters. But those clusters are very homogenous (high non-overlap scores).

5 CONCLUSION

In this paper, we have mainly proposed a comparison between clustering methods: direct vs multilevel, then crisp vs fuzzy/evidential. To enhance the fuzzy/evidential multilevel algorithms, a new split criterion has also been proposed (*Mass a posteriori* split criterion).

Several conclusions were obtained. First, direct methods may result in a bad structure recognition due to particular geometry shapes like nested or close clusters. Agglomerative methods may also be disturbed by connected noisy clusters. This problem also affects HDBSCAN, despite its ability to cluster noise. Moreover, the number of clusters obtained by HDBSCAN can be extremely sensitive to its parameter *minPts* on this type of datasets.

An other shortcoming of agglomerative methods, and spectral clustering as well, is their complexity: they are not suitable for large datasets because of too high computing times.

Multilevel approaches like multilevel C-means or ECM can help to recognize noisy/ambiguous clusters, what's more, in a reasonable computing time. On some datasets, the final clustering appears a lot better than those obtained with direct methods: the ambiguity between clusters may be better processed working with several levels.

Then the comparison of split-criteria leads to the conclusion that those based on soft membership degrees can limit the over-clustering, with a *K*-number closer to the ground truth.

Nevertheless, multilevel approaches based on K-means and its fuzzy/evidential extensions are clearly not perfect. In particular, they are based on a delicate task, the automatic estimation of the cluster number, which is repeated frequently. Their parameters are estimated in order to obtain a final number of clusters close to the known number of classes. Another reason which may disadvantage multilevel methods, is the difficulty to obtain a fair comparison with other clustering methods, when the final number of clusters differs. Split criteria thresholds were chosen to make this number closer to the ground-truth, but it often failed: they tend to overcluster. But, the fuzzy/evidential approach provides ambiguity information on clusters that could be used to perform a fusion and retrieve original classes. The good non-overlapping scores obtained in the experiments tend to support this idea.

Further works will therefore investigate the characterization of points and clusters ambiguity in fuzzy and evidential algorithms, in order to improve each clustering step, and to drive the merger process to the building of a more coherent final clustering tree. Moreover, such an approach would reduce the computing time, by making the spectral embedding step useless.

ACKNOWLEDGMENTS

This work is a part of the JERICO-S3 project, funded by the European Commission's H2020 Framework Programme under grant agreement No. 871153. Project coordinator: Ifremer, France.

REFERENCES

- Azzalini, A. and Menardi, G. (2013). *Clustering Via Non-parametric Density Estimation: the R Package pdf-Cluster*.
- Campello, R. and Hruschka, E. (2006). A fuzzy extension of the silhouette width criterion for cluster analysis. *Fuzzy Sets and Systems*, 157(21):2858–2875.
- Denœux, T. (2021). *evclust: An R Package for Evidential Clustering*. Bananas dataset.
- Gionis, A., Mannila, H., and Tsaparas, P. (2007). Clustering aggregation. *ACM Transactions on Knowledge Discovery from Data*, 1(1):4.
- Grassi, K., Poisson Caillault, E., and Lefebvre, A. (2019). Multilevel spectral clustering for extreme event characterization. In *OCEANS 2019 - Marseille*. IEEE.

- Masson, M.-H. and Dencœur, T. (2007). Algorithme évidentiel des c-moyennes ecm : Evidential c-means algorithm. In *Rencontres Francophones sur la Logique Floue et ses Applications (LFA'07)*, pages 17–24, Nîmes, France, Novembre, 2007.
- McInnes, L., Healy, J., and Astels, S. (2017). hdbscan: Hierarchical density based clustering. *The Journal of Open Source Software*, 2(11):205.
- Mächler, M., Rousseeuw, P., Struyf, A., Hubert, M., and Hornik, K. (2012). *Cluster: Cluster Analysis Basics and Extensions*, R-CRAN packages.
- Ng, A. and Jordan, M. and Weiss, Y. (2001). On Spectral Clustering: Analysis and an algorithm. In *Advances in Neural Information Processing Systems (NIPS'01)*, pages 849–856. MIT Press.
- Sanchez-Garcia, J., Fennelly, M., Norris, S., Wright, N., Niblo, G., Brodzki, J., and Bialek, J. W. (2014). Hierarchical spectral clustering of power grids. *IEEE Transactions on Power Systems*, 29(5):2229–2237.
- Shi, J. and Malik, J. (2000). Normalized cuts and image segmentation. *IEEE Trans. Pattern Anal. Mach. Intell.*, 22(8):888–905.
- Zahn, C. (1971). Graph-theoretical methods for detecting and describing gestalt clusters. *IEEE Transactions on Computers*, C-20(1):68–86.
- Zelnik-manor, L. and Perona, P. (2004). Self-tuning spectral clustering. In Saul, L., Weiss, Y., and Bottou, L., editors, *Advances in Neural Information Processing Systems (NIPS'04)*. MIT Press.

