Comparison of Combination Methods using Spectral Clustering Ensembles

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Abstract. We address the problem of the combination of multiple data partitions, that we call a clustering ensemble. We use a recent clustering approach, known as *Spectral Clustering*, and the classical *K-Means* algorithm to produce the partitions that constitute the clustering ensembles. A comparative evaluation of several combination methods is performed by measuring the consistency between the combined data partition and (a) ground truth information, and (b) the clustering ensemble. Two consistency measures are used: (i) an index based on cluster matching between two partitions; and (ii) an information theoretic index exploring the concept of mutual information between data partitions. Results on a variety of synthetic and real data sets show that, while combination results are more robust solutions than individual clusterings, no combination method proves to be a clear winner. Furthermore, without the use of *a priori* information, the mutual information based measure is not able to systematically select the best combination method for each problem, optimality being measured based on ground truth information.

1 INTRODUCTION

Let $X = \{x_1, x_2, \ldots, x_n\}$ be a set of n objects, and $S = \{s_1, \ldots, s_n\}$ be a set of vectors representing the data in a d-dimensional space, $s_i \in \mathbb{R}^d$. Many clustering algorithms exist, producing distinct partitionings of the data. Let's define *clustering ensemble* as a set of N partitions, $\mathbb{P} = \{P^1, P^2, \ldots, P^i, \ldots, P^N\}$, where each partition, $P^i = \left\{C_1^i, C_2^i, \ldots, C_{k_i}^i\right\}$, has k_i clusters.

Inspired in the work of sensor fusion and classifier combination [1, 2], the idea of combining data partitions produced by multiple algorithms or data representations has recently been proposed [3–5], trying to benefit from the strengths of each algorithm, with the objective of producing a better solution than the individual clusterings.

This framework, known as *Combination of Clustering Ensembles*, has many strong points when compared to individual clustering algorithms, namely: robustness, overcoming instabilities of the individual clustering algorithms and/or avoiding parameter selection; parallelization or distributed partition computation, improving scalability and the ability to deal with distributed clustering. To

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apply this technique, relevant and challenging questions have to be addressed: *How to produce the partitions of the clustering ensemble? How to combine multiple partitions? How to validate the results?*

The clustering ensemble can be produced in many different ways, including: different algorithms [4]; different parameter values/initializations of a single algorithm [6]; clustering different views/features of the data or manipulating the data set, using techniques such as bootstrapping or boosting [7]. In this paper we investigate the effect of combining clusterings produced by a single algorithm with different initialization and/or parameter values. Two algorithms are discussed: the K-means algorithm and a spectral clustering method.

Several combination methods have been proposed to obtain the combined solution, that we will refer as P^* [3, 4, 6, 8–10]. Fred [3] proposed a method for finding consistent data partitions, where combination of clustering results is performed transforming partitions into a co-association matrix, which maps the coherent associations. The combined partition is determined using a majority voting scheme, by applying the single-link algorithm to the co-association matrix. This mapping into a new similarity measure is further explored, by Fred and Jain [6] introducing the concept of Evidence Accumulation Clustering (EAC). Strehl and Gosh [4] have formulated the clustering ensemble problem as an optimization problem based on the maximal average mutual information between the optimal combined clustering and the clustering ensemble. Three heuristics are presented to solve it, exploring graph theoretical concepts. Topchy, Jain and Punch, [8], proposed to solve the combination problem based on a probabilistic model of the consensus partition in the space of clusterings. The consensus partition is found as a solution to the maximum likelihood problem for a given clustering problem. The EM algorithm is used to solve this problem. Other approaches include a collective hierarchical clustering algorithm for the analysis of distributed, heterogeneous data [9] and an unsupervised voting-merging algorithm which deals iteratively with the cluster correspondence problem [10].

In this work we compare three of the above combination methods: evidence accumulation clustering, referred as EAC, by Fred and Jain; the three heuristics by Strehl and Gosh, referred as Graph Based; the probabilistic model, referred as Finite Mixture, by Topchy, Jain and Punch. Section 3, presents these combination strategies. Concerning the EAC combination technique, we further explore other hierarchical clustering methods (Average Link, Complete link, Wards and Centroid based linkage) for the extraction of the final data partition. The types of clustering ensembles used in the study are presented in section 2, comprising results produced by spectral clustering partitioning and the K-means algorithm. Finally, in section 4 a variety of synthetic and real data sets are used to empirically compare the combination techniques. The evaluation of results is based on a consistency index, C_i, between the combined data partition and the "ideal data partition" taken as ground truth information, and on an information theoretic based index that uses the information in the clustering ensemble.

2 PRODUCING CLUSTERING ENSEMBLES

There are many methods employed to generate clustering ensembles. We explore the spectral clustering algorithm by Ng. and al. [11] and the classical K-Means algorithm, selecting different parameters values to obtain the partitions.

2.1 Spectral-based Clustering Ensemble

Spectral clustering algorithms map the original data set into a different feature space based on the eigenvectors of an affinity matrix, a clustering method being applied to the new feature space. Several spectral clustering algorithm exist in the literature [12]. We build on the work by Ng. et Al. [11]. The algorithm described in [11] starts by forming an affinity matrix, $A \in \mathbb{R}^{n \times n}$, defined by

$$A_{ij} = exp(-\|s_i - s_j\|)^2/2\sigma^2 \quad \text{if } i \neq j, \quad \text{and } A_{ii} = 0, \tag{1}$$

where σ is a scaling parameter. Then, the matrix X is formed by stacking the columns corresponding to the K largest eigenvectors of $L(A) = D^{-1/2}AD^{-1/2}$, where D is a diagonal matrix with elements D_{ii} given by the sum of the ith row elements of A. The data partition is obtained by K-means clustering of a matrix, Y, formed by normalizing the rows of the matrix X.

Distinct clusterings are obtained depending on parameter initialization, namely K, the number of clusters, and σ, the scaling parameter controlling the decay of the affinity matrix. We build the spectral clustering ensembles using these parameters in two different ways:

(i) assuming a fixed K, the ensemble $\mathbb{P}$ is obtained by applying the spectral clustering algorithm with σ taking values in a large interval, $[\sigma_{min} : inc : \sigma_{max}]$, where inc represents an increment;
(ii) for each $K \in \mathcal{K} = \{K_1, \ldots, K_m\}$, apply the spectral clustering algorithm with σ varying over the interval $[\sigma_{min} : inc : \sigma_{max}]$.

2.2 K-Means based Clustering Ensemble

In [3], two ways of producing data partitions using the K-Means algorithm, with random initialization of the cluster centers, are explored: (i) using a fixed K value in all partitions, diversity of solutions are mainly due to random initialization of the algorithm; (ii) random selection of K within an interval $[K_{min}; K_{max}]$. In this paper we use the second approach, building an ensemble with $N = 200$ data partitions by randomly initializing the K-means algorithm, with K randomly chosen within the interval [10; 30]. It has been shown that this approach ensures a greater diversity of components in the ensemble and more robust solutions.

3 COMBINING DATA PARTITIONS

The combination methods presented next are based on the mappings of the individual partitions in the clustering ensemble into: a new similarity matrix (EAC); a hypergraph (graph based techniques); or a new feature space of categorical values given by the labels in the partitions (finite mixture method).

3.1 Evidence Accumulation Clustering - EAC

The idea of evidence accumulation clustering [3, 6] is to combine the results of multiple clusterings, by mapping the relationships between pairs of patterns into a $n \times n$ co-association matrix, $\mathcal{C}$. Evidence accumulated over the N clusterings in $\mathbb{P}$ induces the new similarity measure between patterns synthesized in $\mathcal{C}$, according to the equation

$$\mathcal{C}(i,j) = \frac{n_{ij}}{N}, \tag{2}$$

where n_{ij} represents the number of times a given sample pair (i,j) has co-occurred in a cluster over the N clusterings.

The application of the Single-link hierarchical algorithm to the co-association matrix yields the combined data partition P^* in [6]). Here we further explore other hierarchical methods, namely the Average Link (AL), Complete Link (CL), Ward's Link (WL), and the Centroid Linkage (Cent), for extracting the final data partition from the co-association matrix. In this process, the number of clusters could be fixed or automatically chosen using the lifetime criteria described in [6]. For comparison purposes with the other combination methods, we will assume K known.

3.2 Graph Based Clustering

Adopting a graph-theoretical approach, Strehl and Gosh [4] map the clustering ensemble into a hypergraph, where vertices correspond to samples, and partitions are represented as hyperedges. The mapping between each cluster and the hyperedges is performed by means of a binary membership function. Three different heuristics are presented to solve the combination problem. The first heuristic, Cluster-based Similarity Partitioning Algorithm, (CSPA), is similar to the EAC approach, generating a similarity co-association matrix from the hypergraph representation of the partitions. The final partition is obtained using the METIS algorithm [13], viewing the obtained similarity matrix as an adjacency matrix of a graph. The second algorithm, the HyperGraph-Partition Algorithm (HGPA), partitions the hypergraph by cutting a minimum number of hyperedges using the HMETIS package [14]. The last heuristic, the Meta Clustering Algorithm (MCLA), is based on clustering clusters, using hyperedge collapsing operations to reduce the number of hyperedges to K. In all these algorithms, the number of clusters, K, is assumed to be known.

Given the combined partitions produced by the three combination algorithms, P^{*1}, P^{*2}, P^{*3}, the "best" solution is chosen in [4] as the one that has maximum average mutual information with all individual partitions, P^i in $\mathbb{P}$:

$$P^* = \arg\max_{P^{*q}} ANMI(P^{*q}, \mathbb{P}) = \arg\max_{P^{*q}} \frac{1}{N} \sum_{i=1}^{N} NMI(P^{*q}, P^i) \tag{3}$$

where NMI is defined as [4]:

$$NMI(P^i, P^j) = \frac{I(P^j, P^j)}{\sqrt{H(P^i)H(P^j)}} \tag{4}$$

where $H(P^i)$ is the entropy of partition P^i and $I(P^i, P^j)$ is the mutual information between partitions P^i and P^j.

The $ANMI(P, \mathbb{P})$ index will also be used to compare the performance of the other combination methods, using the same clustering ensemble.

3.3 Finite Mixture Approach

Let y_{lj} be the label assigned to the object x_l according to the partition P^j. Consider y_l the vector containing the labels assigned to x_l in all N partitions of the clustering ensemble, $\mathbb{P}$. Topchy et al. [8] assume that the labels y_l are modelled as random variables drawn from a probability distribution described as a mixture of multiple components, that is:

$$P(y_l|\Theta) = \sum_{m=1}^{K} \alpha_m P_m(y_l|\theta_m), \tag{5}$$

where each component is parameterized by θ_m. A conditional independence assumption is made for the components of the y_l vector:

$$P_m(y_l|\theta_m) = \prod_{j=1}^{N} P_m^{(j)}(y_{lj}|\theta_m^{(j)}) \tag{6}$$

Then $P_m^{(j)}(y_{lj}|\theta_m^{(j)})$ is chosen as an outcome of a multinomial trial:

$$P_m^{(j)}(y|\theta_m^{(j)}) = \prod_{k=1}^{k_j} \vartheta_{jm}(k)^{\delta(y,k)}, \tag{7}$$

where k_j is the number of clusters in partition P^j, $\delta(y, k) = 1$ if $y = k$ and $\delta(y, k) = 0$ otherwise.

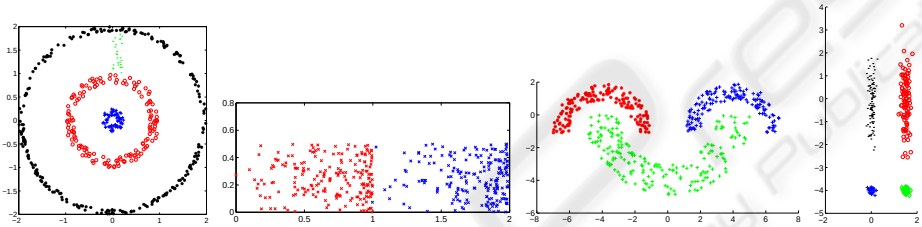
The EM algorithm is used to simultaneous handle the unknown class and model problem. A new variable $z_l = z_{l1}, \ldots, z_{lK}$ is associated as hidden variable, such that $z_{lm} = 1$ if y_l belongs to the m-th component of the mixture and $z_{lm} = 0$ otherwise.

We assumed that the mixing coefficients α_m, which correspond to the prior probability of the cluster, were equally likely in the first iteration. Furthermore the values $P_m^{(j)}(y_{ij}|\theta_m^{(j)})$ and ϑ were randomly initialized. The EM convergence criteria is based on the variance of $E(z_{im})$, that represents the probability of the pattern y_i being generated by the m-th mixture. The final data partition is obtained assigning to each x_i the model with the largest value of the hidden value (z_m). Due to the risk of convergence of the EM algorithm to a solution of lower quality the authors proposed to pick the best of 3 independent runs. The objective function used for that purpose is the likelihood $L(\Theta|Y, Z)$.

4 EXPERIMENTAL RESULTS AND DISCUSSION

4.1 Data Sets

Synthetic Data Sets For simplicity of visualization, synthetic data sets consist of 2-dimensional patterns. Data sets were generated in order to evaluate the performance of the combination algorithms in a variety of situations, such as arbitrary shaped clusters, distinct data sparseness in the feature space,well separated and touching clusters. Figure 1 plots these data sets. The Rings data set, consists of 500 samples organized in 4 classes (with 25,75,150 and 250 patterns each). The Bars data set is composed by 2 classes (200,200), the density of the patterns increasing with increasing horizontal coordinate. The Half Rings data set has 3 uniformly distributed classes (150-150-200) within half-ring envelops. The Cigar data set has 4 classes (with 100,100,25 25 patterns each).



(a) Rings. (b) Bars. (c) Half Rings. (d) Cigar.

Fig. 1. Synthetic Data Sets.

Real Data Sets The first real application concerns DNA microarrays. The yeast cell data consists of the fluctuations of the gene expression levels of over 6000 genes over two cell cycles. The available data set is restricted to the 384 genes (http://staff.washington.edu/kayee/model/) who's expression level peak at different time points corresponding to the 5 phases of the cell cycle. We used the logarithm of the expression level and a "standardized" version of the data (with mean zero and variance 1) as suggested in [15]. The clustering process should join the expression levels corresponding to the 5 phases of the cell cycles.

The second real data set, Handwritten Digits, is available at the UCI repository (http://www.ics.uci.edu/∼mlearn/MLRepository.html). From a total of 3823 available training samples (each with 64 features) we used a subset composed by the first 100 samples of all the digits [12].

4.2 Combination of Clustering Ensembles Produced by K-Means and Spectral clustering

To evaluate the performance of the combination methods, we will compare the combined data partitions, P^*, with ground truth information, P^o, obtained from known labelling of the data. We will assume that the true number of clusters, K, is known, being the number of clusters in P^*. We use the consistency index proposed in [3] to assess the quality of a clustering, $C_i(P^*, P^o)$; it is defined

as the fraction of shared samples in matching clusters of P^* and P^o. When data partitions have the same number of clusters, $C_i(P^*, P^o)$ is equal to the percentage of correct labelling.

			EAC					Graph			Finite Mixture			
Data Set		K_i	SL	CL	AL	WL	Cent	CSPA	HGPA	MCLA	Max	Mean	STD	L
Rings	Spectral	3	61.4	44.6	48.4	48.4	48.4	45.0	25.4	41.6	61.8	46.5	9.0	**61.8**
		4	47.6	51.4	50.0	50.4	50.0	**63.2**	25.4	43.0	85.8	54.3	13.0	49.8
		20	80.0	40.0	**81.8**	79.6	59.8	70.4	72.8	59.2	55.0	47.3	6.0	45.6
		All	**80.4**	46.0	50.8	48.2	46.2	67.0	51.6	50.4	62.0	46.0	6.0	50.2
	Kmeans	All	**85.6**	40.0	44.6	59.4	51.0	47.8	67.2	61.2	60.60	50.30	8.00	59.4
	Dist		58.8	36.8	34.0	43.4	43.6							
Half Rings	Spectral	3	64.6	85.8	86.2	**87.6**	86.2	83.2	45.4	84.6	85.2	68.7	9.0	83.2
		8	69.8	41.2	**97.2**	92.8	58.2	93.4	92.6	95.0	72.8	56.7	9.0	62.6
		All	**95.0**	87.6	**95.0**	**95.0**	**95.0**	93.2	89.2	93.0	74.6	58.6	12.0	51.0
	Kmeans	All	**99.8**	38.2	95.0	95.0	51.6	93.4	95.0	93.8	56.60	46.30	6.00	56.6
	Dist		95.0	72.0	73.4	73.6	73.6							
Cigar	Spectral	4	**100.0**	**100.0**	**100.0**	**100.0**	**100.0**	71.2	34.4	**100.0**	100.0	88.8	11.0	**100.0**
		5	**100.0**	61.6	**100.0**	**100.0**	**100.0**	70.8	41.2	73.6	100.0	81.8	9.0	**100.0**
		8	**100.0**	61.6	**100.0**	70.4	79.6	70.0	70.4	66.8	72.8	59.4	8.0	58.8
		All	**100.0**	**100.0**	**100.0**	**100.0**	**100.0**	70.4	74.8	63.2	54.0	44.8	7.0	44.4
	Kmeans	All	**100.0**	64.0	71.0	70.0	67.0	60.0	73.0	61.0	74.40	51.60	11.00	74.4
	Dist		60.4	55.6	87.2	58.0	51.6							
Bars	Spectral	2	96.8	96.8	96.8	96.5	96.8	**99.0**	50.0	96.8	97.0	96.7	0.3	96.8
		15	**99.5**	55.0	**99.5**	**99.5**	55.8	99.2	97.0	**99.5**	80.5	62.9	10.0	80.5
		All	**98.8**	97.5	97.5	**98.8**	97.5	97.8	**98.8**	**98.8**	75.5	59.4	8.0	75.5
	Kmeans	All	54.3	55.5	98.8	98.8	57.5	**99.0**	98.0	**99.0**	79.30	63.00	10.00	74.2
	Dist		50.2	98.8	98.8	99.5	99.5							
Log Yeast	Spectral	4	31.5	25.8	33.6	36.2	34.1	35.2	22.1	36.2	37.2	35.5	1.0	**37.2**
		5	34.4	41.9	37.2	37.8	37.2	34.9	31.3	**44.5**	37.8	34.0	4.0	34.4
		6	34.6	33.1	38.3	**39.3**	38.3	36.2	30.7	38.0	46.6	35.9	7.0	33.6
		20	35.9	34.4	**45.3**	37.8	37.5	35.4	40.1	39.3	44.0	39.7	3.0	36.2
		All	34.4	30.2	36.5	36.5	35.7	32.6	29.2	32.8	44.3	42.0	2.00	**40.4**
	KMeans	All	37.0	27.0	**41.0**	35.0	41.0	34.0	32.0	32.0	39.80	36.40	3.00	36.20
	Dist		34.9	28.9	28.6	35.9	30.7							
Std Yeast	Spectral	4	35.7	66.7	66.4	64.3	**66.9**	60.4	38.0	66.1	64.6	59.8	5.0	64.6
		5	49.2	57.3	**66.1**	65.4	**66.1**	59.4	38.8	64.3	65.9	59.6	6.0	65.9
		6	45.6	61.5	**68.2**	65.4	**68.2**	56.5	37.2	67.2	63.8	57.8	5.0	60.9
		20	36.2	43.2	**62.8**	52.3	39.3	55.5	56.5	59.1	60.9	54.3	6.0	57.0
		All	44.8	65.6	**65.9**	65.4	65.1	56.8	59.4	58.9	64.1	52.8	12.0	64.1
	KMeans	All	48.0	54.0	**67.0**	56.0	45.0	53.0	57.0	54.0	51.60	45.20	8.00	39.30
	Dist		36.2	66.7	65.9	66.9	57.8							
Optical	Spectral	9	60.5	79.0	77.3	**84.3**	77.3	79.5	35.2	79.5	77.1	65.3	9.0	77.1
		10	70.0	77.3	77.6	**84.5**	77.6	80.5	33.4	**84.5**	75.6	69.7	6.0	67.9
		15	72.2	53.0	72.2	**88.3**	73.8	86.3	52.7	78.1	75.9	67.4	8.0	75.9
		All	60.4	75.0	79.1	87.3	79.1	**88.1**	45.4	77.1	72.6	67.8	4.0	72.6
	Kmeans	All	40.0	51.0	79.0	80.0	71.0	84.0	78.0	**88.0**	64.00	57.90	4.00	54.30
	Dist		10.6	54.1	75.7	74.8	10.6							

Table 1. Combination Results - $C_i(P^*, P^o)$ - for Spectral and K-means Clustering Ensembles. Best results for each clustering ensemble are represented in **bold** style.

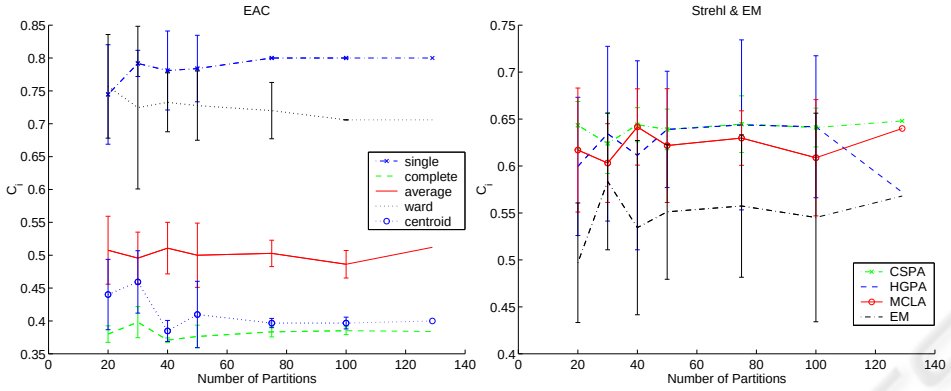
Table 1 shows the $C_i(P^*, P^o)$ index for spectral and K-means clustering ensembles with both synthetic and real data sets (see first column). In this table, rows are grouped by clustering ensemble construction method (second column). Rows corresponding to Spectral Clustering Ensembles, with numerical labels in the K_i column indicate that the clustering ensemble has only partitions with K_i clusters (method (i) in section 2.1). For each K, a clustering ensemble with $N = 22$ data partitions was produced by assigning σ values between 0.08 and 0.5, with increments of 0.02 (schematically described by the notation [0.08:0.02:0.5]). We have tested with K taking all the values in the set $\mathcal{K} = \{2, 3, 4, 5, 6, 7, 8, 9, 10, 15, 20\}$; due to space limitations, only a small number of experimental results are presented. Rows corresponding to Spectral Clustering Ensembles, with the label "All" (method (ii) in section 2.1) correspond to the union of all the partitions produced by method (i) with K taking all the values

in the set $\mathcal{K}$ ($N = 242$). For the K-means ensemble the row "All" represents the results obtained with N=200, and K randomly chosen in the set $\{10, \ldots, 30\}$. Finally the rows "Dist" represent the results obtained by each of the hierarchical clustering methods directly applied to the Euclidean distance matrix between objects in the original feature space.

Columns are grouped by combination method. Corresponding to the EAC method, columns with titles "SL", "CL", "AL", "WL" and "Cent" represent the methods of extraction of the final data partition, respectively: Single Link, Complete link, Average link, Wards Link and Centroid Linkage. The Graph based strategy has three columns corresponding to the heuristics "CSPA", "HGPA" and "MCLA". Computation of these results used the Matlab implementation made available at (http://strehl.com). The last method - Finite Mixture - is characterize by columns "Max", "Mean, "STD" and "L", representing the maximum, the mean, and standard deviation of the consistency index over 10 runs of EM algorithm (for the real data sets only 5 runs were used); column L represents the best run using the established criteria (likelihood).

From the analysis of table 1 we see that none of the methods is a clear winner (each combination method produces best results at least once). Observation of the clusters structure help to enlighten which method is more suitable for each situation. When dealing with arbitrary shaped, well separated clusters, such as in the Half Rings and the Cigar data sets, the EAC method performed better than the others; the superiority of the SL variation of the EAC method is here particularly evident when comparing results with clustering ensembles produced by the K-means algorithm, as the spectral clustering algorithm maps the original feature space to another space where clusters are more compactly represented, and therefore clustering algorithms favoring compacticity should work well. In situations of touching clusters (Rings and Bars), the Graph based heuristics have a performance similar to EAC. In the real data sets the performance is very good compared with the results presented in [12], where for Optical Digits the best result was about 20% of clustering error, and with the combination of clusterings the best error rate achieved is about 10%. For the log-normalized yeast cell data the results were worst than in [12], where clustering error is about 40% compared with the 55% in the present work. Finally for the standardized yeast cell data in [12] the clustering error was 35%, which is comparable to the best error rate present in table 1.

Comparison of K-means based and spectral clustering based combination results show that the combination of clustering ensembles produced by the spectral clustering algorithm leads, in general, to better data partitions (at the expense of a higher computational burden); when dealing with well separated clusters, both methods of constructing the clustering ensemble lead to comparable results, the K-means approach being a more adequate choice due to its low computational complexity. Application of the hierarchical clustering algorithms directly to the Euclidean distances between patterns lead, most of the times, to the poorest performances observed.



(a) EAC. (b) HyperGraph and Finite Mixture.

Fig. 2. Evolution of mean values and standard deviation of $C_i(P^*, P^o)$ as a function of N, the number of partitions in the clustering ensemble, for the Rings data set; the clustering ensemble was created using the spectral clustering algorithm with $K = 15$ and σ =[0.08:0.01:0.99 1:.25:10].

Another interesting comparison between the methods concerns the rate of convergence and stability of the combination solutions as a function of N, the cardinality of the clustering ensemble. We have observed that the EAC method leads to better convergence curves, the variance of the consistency index $C_i(P^*, P^o)$, as computed over 10 repetitions of the combination experiment, decreasing to zero, a value that is achieved with $N < 200$ in all data sets under study. Figure 2 illustrates the results of the $C_i(P^*, P^o)$ for the the Rings data set, using spectral clustering with $K = 15$, and randomly picking partitions obtained with σ in set [0.08:0.01:0.99 1:.25:10]. As the number of partitions grows, the standard deviation of $C_i(P^*, P^o)$ for the EAC methods diminish, the combined partition converging to a unique solution (null variance) with $N < 120$; the other combination methods, however, with the exception of CSPA, present not so stable solutions, exhibiting large variances of results over the entire interval for N.

4.3 Selection of the Combination Method

We have empirically demonstrated in the previous section that none of the combination methods under study proves to be the best for all situations, results depending on the data sets, and on the way of producing the clustering ensemble. Strehl and Gosh [4] proposed to use the average normalized mutual information - $ANMI(P^*, \mathbb{P})$ (see section 3.2) - as criteria for selecting among the combination results produced by different combination strategies. We now compare the several methods based on this consensus measure, and investigate its usefulness for the selection of the combination method.

Table 2 presents the values of $ANMI(P^*, \mathbb{P})$ for the data sets and combination methods in correspondence with table 1, exception made for the Finite

Mixture column that corresponds to column L in table 1. It is easy to see that none of the methods gives overall best consensus with the clustering ensemble: highest $ANMI(P^*, \mathbb{P})$ values are distributed along all columns in this table.

Data Set	K_i	SL	CL	AL	WL	Cent	CSPA	HGPA	MCLA	Finite Mixture (L)
Rings	3	0.448	0.609	0.606	0.607	0.606	0.517	0.003	0.602	0.605
	4	0.655	0.789	0.798	0.799	0.798	0.610	0.007	0.740	0.717
	20	0.553	0.228	0.621	0.513	0.363	0.619	0.631	0.604	0.573
	All	0.511	0.553	0.630	0.632	0.635	0.511	0.483	0.629	0.311
	kmeans	0.5693	0.3666	0.5791	0.4910	0.2943	0.5693	0.5840	0.5768	0.3954
Half Rings	3	0.666	0.843	0.842	0.833	0.842	0.831	0.187	0.842	0.844
	8	0.392	0.364	0.598	0.579	0.403	0.581	0.594	0.603	0.530
	All	0.609	0.610	0.609	0.609	0.609	0.599	0.608	0.610	0.524
	kmeans	0.5234	0.2185	0.5380	0.5380	0.2323	0.5201	0.5380	0.5277	0.2370
Cigar	4	0.994	0.994	0.994	0.994	0.994	0.669	0.120	0.994	0.994
	5	0.908	0.641	0.908	0.908	0.908	0.693	0.177	0.814	0.908
	8	0.753	0.519	0.753	0.777	0.678	0.704	0.722	0.762	0.723
	All	0.750	0.750	0.750	0.750	0.750	0.609	0.615	0.675	0.451
	kmeans	0.5941	0.5412	0.6401	0.6400	0.4553	0.6115	0.6249	0.5962	0.4308
Bars	2	0.974	0.974	0.974	0.969	0.974	0.852	<0.001	0.974	0.974
	15	0.395	0.094	0.395	0.395	0.144	0.389	0.394	0.395	0.338
	All	0.543	0.545	0.545	0.543	0.545	0.516	0.543	0.543	0.236
	kmeans	0.0817	0.1089	0.3816	0.3816	0.1462	0.3661	0.3812	0.3816	0.2508
Log Yeast	4	0.052	0.615	0.662	0.652	0.662	0.565	0.422	0.659	0.645
	5	0.050	0.596	0.590	0.604	0.614	0.558	0.487	0.576	0.543
	6	0.049	0.521	0.600	0.580	0.560	0.545	0.537	0.561	0.536
	20	0.341	0.349	0.562	0.565	0.200	0.531	0.551	0.544	0.483
	All	0.064	0.503	0.537	0.539	0.494	0.520	0.428	0.525	0.351
	kmeans	0.3165	0.4192	0.6143	0.6041	0.3041	0.6011	0.6001	0.6065	0.3697
Std Yeast	2	0.492	0.632	0.753	0.757	0.755	0.693	0.287	0.753	0.721
	3	0.029	0.633	0.720	0.710	0.722	0.664	0.304	0.721	0.670
	4	0.345	0.630	0.708	0.707	0.707	0.654	0.391	0.660	0.687
	5	0.062	0.202	0.590	0.570	0.188	0.571	0.566	0.565	0.511
	All	0.332	0.625	0.659	0.655	0.657	0.616	0.511	0.623	0.523
	kmeans	0.4202	0.4720	0.6304	0.6489	0.3595	0.6325	0.6487	0.6386	0.4633
Optical	9	0.844	0.921	0.944	0.933	0.944	0.867	0.425	0.910	0.885
	10	0.829	0.928	0.937	0.929	0.937	0.855	0.388	0.928	0.890
	15	0.878	0.783	0.907	0.921	0.883	0.855	0.590	0.878	0.861
	All	0.766	0.758	0.754	0.741	0.754	0.699	0.463		0.595
	kmeans	0.4803	0.6144	0.7850	0.7819	0.7680	0.7567	0.7338	0.7782	0.6065

Table 2. Values of the consensus function $ANMI(P^*, \mathbb{P})$ for the data sets and situations in table 1.

Comparison of best results according to the consistency measure with ground truth information, $C_i(P^*, P^o)$, in table 1 with the consensus measure with the clustering ensemble, $ANMI(P^*, \mathbb{P})$, in table 2 leads to the conclusion that there is no correlation between these two measures; therefore, the mutual information based consensus function is not suitable for the selection of the best performing method in each situation.

5 Conclusions

In this work we addressed the problem of combining multiple data partitions in the context of spectral clustering and k-means clustering. Clustering ensembles were either produced by using the K-means algorithm or the spectral clustering algorithm by Ng et al [11], with different parameter values and/or different initializations. Three different combination strategies found in the literature, namely evidence accumulation clustering, graph based combination and maximum likelihood combination (finite mixture model), were compared and analyzed empirically. Test data sets consisted both on synthetic data, illustrating different cluster structures, and real application data. For each data set, and each

clustering ensemble, the several combination algorithms, and variants herein proposed, were applied in order to obtain the combined data partition P^*. Using known labelling of the data - ideal partition P^o - as ground truth information, a consistency index between the combined data partition, P^*, and P^o ($C_i(P^*, P^o)$) was computed. Comparison of the several combination methods using this consistency index has shown that there is no best method for all situations, results depending on the data sets and on the way of building the clustering ensembles. The finite mixture model seems to be more appropriate for situations with clustering ensembles with a few number of partitions where the number of clusters in each partition is near the true number of clusters. The other methods (EAC and Graph based) seem more robust and can better handle most situations. Analysis of the variance of the consistency measure, computed over multiple runs of the experiments, has shown that the evidence accumulation strategy leads to more stable results, converging to a unique combination solution (null variance of $C_i(P^*, P^o)$) when the cardinality of the clustering ensemble, N, is sufficiently large, typically with $N < 200$; the other techniques exhibit, most of the times, a large variance for the consistency index. The problem of selecting amongst the combination results was also addressed using the mutual information based consensus measure proposed by Strehl and Gosh [4], measuring the consensus between the combined partition and the clustering ensemble. Experimental results demonstrated that this measure is not adequate for selecting the best performing method, as there is no correspondence between best consensus values and consistency with ground truth information.

Ongoing work include the investigation of criteria for the comparison and selection of best combination techniques.

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