Evidence Accumulation Clustering using Pairwise Constraints

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Abstract: Recent work on constrained data clustering have shown that the incorporation of pairwise constraints, such as must-link and cannot-link constraints, increases the accuracy of single run data clustering methods. It was also shown that the quality of a consensus partition, resulting from the combination of multiple data partitions, is usually superior than the quality of the partitions produced by single run clustering algorithms. In this paper we test the effectiveness of adding pairwise constraints to the Evidence Accumulation Clustering framework. For this purpose, a new soft-constrained hierarchical clustering algorithm is proposed and is used for the extraction of the consensus partition from the co-association matrix. It is also studied whether there are advantages in selecting the must-link and cannot-link constraints on certain subsets of the data instead of selecting these constraints at random on the entire data set. Experimental results on 7 synthetic and 7 real data sets have shown the use of soft constraints improves the performance of the Evidence Accumulation Clustering.

1 INTRODUCTION

Data clustering is an unsupervised learning discipline which aims to discover structure in data. A clustering algorithm groups a set of unlabeled data patterns into meaningful clusters using some notion of similarity between data, so that similar patterns are placed in the same cluster and dissimilar patterns are assigned to different clusters.

Inspired by the success of the supervised classifier ensemble methods, many unsupervised clustering ensemble methods were proposed in the last decade. The idea is to combine multiple data partitions to improve the quality and robustness of data clustering (Fred, 2001), to reuse existing data partitions (Strehl and Ghosh, 2003), and to partition data in a distributed way. The clustering ensemble methods can be categorized according to the way the clustering ensemble is build: one or several clustering algorithms can be applied, using different parameters and initializations (Fred and Jain, 2005), finding a median partition (Topchy et al., 2003), and mapping the clustering ensemble problem into graph (Fern and Brodley, 2004; Domeniconi and Al-Razgan, 2009) or hypergraph (Strehl and Ghosh, 2003) formulations.

Recently, some researchers focused on including some a priori knowledge about the data into clustering (Basu et al., 2008). Constrained data clustering maps this knowledge as constraints to be used by a constrained clustering algorithm. These constraints manifest the preferences, limitations or conditions that a user may want to impose in the clustering solution, so that the clustering solution may be more useful for each particular case. Some constrained data clustering algorithms have already been proposed regarding distinct perspectives: inviolable constraints (Wagstaff, 2002), distance editing (Klein et al., 2002), using partial label data (Basu, 2005), penalizing the violation of constraints (Davidson and Ravi, 2005), modifying the generation model (Basu, 2005), and encoding constraints into spectral clustering (Wang and Davidson, 2010).

In this paper, we explore the use of pairwise constraints in the Evidence Accumulation Clustering framework. A constrained clustering algorithm is proposed and used to produce consensus partitions. The effect of acquiring constraints involving objects easy
and/or hard to cluster is also investigated.

The remaining of the paper is organized as follows. In section 2, the clustering combination problem and the Evidence Accumulation Clustering method are described in subsection 2.1, the incorporation of constraints in Evidence Accumulation Clustering is explained in subsection 2.2, and ansoft-constrained hierarchical clustering algorithm is proposed in subsection 2.3. The process of acquiring pairwise constraints is presented in section 3. In section 4 the experimental setup of our work is described and the experimental results are presented. Section 6 concludes this paper.

2 EVIDENCE ACCUMULATION CLUSTERING USING PAIRWISE CONSTRAINTS

2.1 Combination of Multiple Data Partitions

Let \( X = \{x_1, \ldots, x_n\} \) be a data set with \( n \) data patterns. A clustering algorithm divides the data set \( X \) into \( K \) clusters resulting in a data partition \( P = \{C_1, \ldots, C_K\} \). By changing the algorithm parameters and/or initializations different partitions of \( X \) can be obtained. A clustering ensemble \( \mathcal{P} = \{P^1, \ldots, P^N\} \) is defined as a set of \( N \) data partitions of \( X \). Consensus clustering methods, also known as clustering combination methods, use the information contained in \( \mathcal{P} \) to produce a consensus partition \( P^c \).

One of the most known clustering combination methods is the Evidence Accumulation Clustering method (EAC) (Fred and Jain, 2005). EAC treats each data partition \( P^l \in \mathcal{P} \) as an independent evidence of data organization. The key idea is that if two data patterns are frequently co-assigned to the same clusters in \( \mathcal{P} \) than they probably belong to the same “natural” cluster.

EAC uses a \( n \times n \) co-association matrix \( C \) to keep the frequency that each pair of patterns is grouped into the same cluster. The co-association matrix is computed as

\[
C_{ij} = \frac{\sum_{l=1}^{N} \text{vote}_{ij}^l}{N},
\]

where \( \text{vote}_{ij}^l = 1 \) if \( x_i \) and \( x_j \) co-occur in a cluster of data partition \( P^l \) and \( \text{vote}_{ij}^l = 0 \) otherwise. After the co-association matrix have been computed, it is used as input to a clustering algorithm to produce the consensus partition \( P^c \).

2.2 Clustering with Constraints

Different types of constraints can be used to influence the data clustering solution. At a more general level, constraints may be applied to the entire data set. An example of this type of constraints is data clustering with obstacles (Tung et al., 2000). The constraints may be used at an intermediate level, where they may be applied to mold the characteristics of the clusters, such as the minimum and maximum capacity (Ge et al., 2007), or to data features (Wagstaff, 2002).

At a more specific level, the constraints may be employed at the level of the individual data patterns, using labels on some data (Basu, 2005) or defining relations between pairs of patterns (Wagstaff, 2002), such as must-link and cannot-link constraints. We will focus on these relations between pairs of patterns due to their versatility: many constraints on more general levels can easily be converted to must-link and cannot-link constraints.

The relations between pair of clusters are represented by two sets: the set of must link constraints (\( \mathcal{R}_{\text{m}} \)) and the set of cannot-link (\( \mathcal{R}_{\text{c}} \)) constraints. On one hand, to indicate that two data patterns, \( x_i \) and \( x_j \), should belong to the same cluster a must-link constraint between \( x_i \) and \( x_j \) should be added to \( \mathcal{R}_{\text{m}} \). On the other hand, if \( x_i \) should not be placed in the cluster of \( x_j \) a cannot-link constraint should be added to \( \mathcal{R}_{\text{c}} \). These instance level constraints can be regarded as hard or soft constraints, whether the constraint satisfaction is mandatory or not.

To incorporate pairwise constraints in the Evidence Accumulation Clustering framework, we simply apply a pairwise-constrained clustering algorithm to the co-association matrix, as suggested in (Duarte et al., 2009). For this purpose, a modification to the average-link (Sokal and Michener, 1958) algorithm is proposed in subsection 2.3. Figure 1 summarizes the Constrained Evidence Accumulation Clustering model. In the first step, the Clustering Generation Step, one or several clustering algorithms using different parameters and initializations are used to produce \( N \) partitions of the given data set. Then, in the Consensus Step, the co-association matrix is built as described in subsection 2.1, and a constrained clustering algorithm uses the information contained in the co-association matrix and the set of pairwise constraints to produce the consensus partition.

2.3 Soft-Constrained Average-link Clustering Algorithm

An agglomerative hierarchical clustering algorithm starts with \( n \) clusters, where each cluster is composed
of a single data pattern, i.e. \( \forall x_i \in X, C_i = \{ x_i \} \). Then, iteratively, the two closest clusters according to some distance measure between clusters are merged. The process repeats until all data patterns belong to the same cluster or some stopping criteria is met (e.g. maximum number of clusters reached). The hierarchy produced by an agglomerative clustering algorithm is usually presented as a dendrogram. An example of a dendrogram is given in figure 2.

Average-link (Sokal and Michener, 1958) is an agglomerative hierarchical clustering algorithm which measures the distance between two clusters as the average distance between all pairs of patterns belonging to different clusters. Equation 2 defines the distance between pairs of clusters:

\[
d(C_k, C_l) = \frac{\sum_{i=1}^{\left| C_k \right|} \sum_{j=1}^{\left| C_l \right|} \text{dist}(x_i, x_j)}{|C_k||C_l|}, \tag{2}
\]

where \( |\cdot| \) is the cardinality of a set.

We propose the following modification to the distance function presented in equation 2 in order to handle the must-link and cannot-link sets of constraints as preferences to be considered while producing the consensus partition:

\[
d(C_k, C_l) = \frac{\sum_{i=1}^{\left| C_k \right|} \sum_{j=1}^{\left| C_l \right|} \text{dist}(x_i, x_j) - \sum_{i=1}^{\left| C_k \right|} \sum_{j=1}^{\left| C_l \right|} I_R(x_i, x_j) + \sum_{i=1}^{\left| C_k \right|} \sum_{j=1}^{\left| C_l \right|} I_R^{-1}(x_i, x_j)}{|C_k||C_l|}, \tag{3}
\]

where \( I_R(x_i, x_j) = 1 \) if \( (x_i, x_j) \in R_m \) and 0 otherwise, and \( p \geq 0 \) is a user parameter that influences the “softness” of the constraints. If \( p = 0 \) the algorithm is equivalent to the Average-link. If \( p \to \infty \) the algorithm will become similar to an hard-constrained Average-link. The idea for the soft-constrained distance function is simple: the distance between clusters should be shrunk for each must-link constraint that will be satisfied by joining the two clusters; and for each cannot-link constraint that would become unsatisfied, the distance between clusters should increase.

3 ACQUIRING MUST-LINK AND CANNOT-LINK CONSTRAINTS

The simplest scheme for acquiring must-link and/or cannot-link constraints consists of iteratively selecting two random data patterns, \( (x_i, x_j) \in X \) and ask the user if the patterns should or should not be placed in the same cluster. If the user answered positively then a must-link constraint is added to the set of must-link constraints, i.e. \( R_m = R_m \cup \{ (x_i, x_j) \} \). Otherwise, a cannot-link constraint is added to the set of must-link constraints \( R_c = R_c \cup \{ (x_i, x_j) \} \). The pro-
process stops when a pre-specified number of constraints is achieved. We call this process Random Acquisition of Constraints (RAC).

Another possibility for acquiring the sets of constraints consists of randomly select a subset of the data patterns and ask the user the cluster label for each pattern. Then, for each possible pair of patterns \((x_i, x_j)\) in that subset a must-link constraint is added to \(\mathcal{R}_c\) if the label of both patterns is the same \((P_i = P_j)\). Otherwise, \((x_i, x_j)\) is added to \(\mathcal{R}_e\). This process will be referred as Random Acquisition of Labels (RAL).

In this paper, we will study another three variations of RAC and RAL processes, based on the confidence of assigning a data pattern to its cluster. We use the information contained in the co-association matrix \(C\) to estimate the degree of confidence of assigning a pattern \(x_i\) to its cluster \(C_k\). On one hand, if the average similarity between \(x_i\) and the other patterns belonging to its cluster \((\{x_j : x_j \in C_k\})\) is higher than the average similarity between \(x_i\) and the patterns belonging to the remaining closest cluster, it is expected that \(x_i\) was well clustered. On the other hand, if the similarity to the remaining closest cluster is higher than the similarity to its cluster, \(x_i\) may have been improperly assigned. The degree of confidence \(\text{conf}(x_i)\) of assigning a pattern \(x_i\) to its cluster \(C_P\) is defined as:

\[
\text{conf}(x_i) = \frac{\sum_{j \in \{x_j \mid x_j \in C_k\}} C_{ij}}{|C_P| - 1} - \max_{1 \leq k \leq K, k \neq P_i} \frac{\sum_{j \in C_k} C_{ij}}{|C_k|}.
\]

Figure 3 exemplifies the degree of confidence \(\text{conf}(x_i)\) for each data pattern belonging to the Half Rings data set. Big (and red) points correspond to data patterns with high confidence, and small (and blue) points to data patterns with low confidence.

It may be beneficial to the quality of constrained data clustering choosing only the patterns with more confidence, less confidence, or a mixture of the two above, in the RAC and RAL processes instead of using all the patterns in a data set.

Let \(X^o\) be the ordered set of \(X\) in ascending order of degree of confidence, i.e., \(X^o = \{x_1^o, x_2^o, \ldots, x_n^o\}\), \(\text{conf}(x_1^o) \leq \text{conf}(x_2^o) \leq \cdots \leq \text{conf}(x_n^o)\).

To investigate the previous hypothesis we propose to apply the RAC and RAL process using a subset \(X'\) of size \(m < n\) of \(X\) using one of the following three criteria:

1. the subset with \textit{lowest} degree of confidence (LRAC and LRAL): \(X' = \{x_1^o, \ldots, x_m^o\}\);
2. the subset with \textit{highest} degree of confidence (HRAC and HRAL): \(X' = \{x_m^o, \ldots, x_n^o\}\);
3. the subset of the \([1/m]\) patterns with \textit{lowest} confidence and the \([m/2]\) patterns with \textit{highest} confidence (LHRAC and LHRAL): \(X' = \{x_1^o, \ldots, x_n^o, x_{m-n+1}^o, \ldots, x_m^o\}\).

### 4 EXPERIMENTAL SETUP AND RESULTS

7 synthetic and 7 real data sets were used to assess the performance of the proposed approach on a wide variety of situations, such as data sets with different cardinality and dimensionality, arbitrary shaped clusters, well separated and touching clusters and distinct cluster densities.

Table 1 presents the summary (number of data patterns \(n\), number of dimensions \(d\) and the number of data patterns for each cluster) of all data sets used in our experiments and Figure 4 illustrates
the 2-dimensional synthetic data sets used in our experiments. A brief description for each real data set is given next. The real data sets used in our experiments are available at UCI repository (http://mlearn.ics.uci.edu/MLRepository.html). The Iris data set consists of 50 patterns from each of three species of Iris flowers (setosa, virginica and versicolor) characterized by four features. One of the clusters is well separated from the other two overlapping clusters. Breast Cancer data set is composed of 683 data patterns characterized by nine features and divided into two clusters: benign and malignant. Yeast Cell data set consists of 384 patterns described by 17 attributes, split into five clusters concerning five phases of the cell cycle. There are two versions of this data set, the first one is called Std Yeast and is a “standardized” version of the same data set, with mean 0 and variance 1. Optdigits is a subset of Handwritten Digits data set containing only the first 100 objects of each digit, from a total of 3823 data patterns characterized by 64 attributes. The House Votes data set is composed of two clusters of votes for each of the U.S. House of Representatives Congressmen on the 16 key votes identified by the Congressional Quarterly Almanac. From a total of 435 (267 democrats and 168 republicans) only the first 100 objects of each digit, from a total of 3823 data patterns characterized by 64 attributes. The Wine data set consists of the results of a chemical analysis of wines grown in the same region in Italy divided into three clusters with 59, 71 and 48 patterns described by 13 features.

Table 1: Data sets overview.

<table>
<thead>
<tr>
<th>Data sets</th>
<th>n</th>
<th>z</th>
<th>K</th>
<th>Cluster Distribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bars</td>
<td>400</td>
<td>2</td>
<td>2</td>
<td>2±100±200</td>
</tr>
<tr>
<td>Circs</td>
<td>400</td>
<td>2</td>
<td>3</td>
<td>2±100±200</td>
</tr>
<tr>
<td>D2</td>
<td>200</td>
<td>2</td>
<td>4</td>
<td>116±39±21±24</td>
</tr>
<tr>
<td>D3</td>
<td>200</td>
<td>2</td>
<td>5</td>
<td>98±23±23±35±21</td>
</tr>
<tr>
<td>Half Rings</td>
<td>400</td>
<td>2</td>
<td>2</td>
<td>2±200</td>
</tr>
<tr>
<td>Rings</td>
<td>500</td>
<td>2</td>
<td>4</td>
<td>75±150±250±25</td>
</tr>
<tr>
<td>Two Clusters</td>
<td>1000</td>
<td>2</td>
<td>2</td>
<td>2±500</td>
</tr>
<tr>
<td>Wine</td>
<td>198</td>
<td>15</td>
<td>3</td>
<td>59±31±48</td>
</tr>
<tr>
<td>Yeast Cell</td>
<td>384</td>
<td>17</td>
<td>5</td>
<td>67±135±75±52±55</td>
</tr>
<tr>
<td>Optdigits</td>
<td>1000</td>
<td>64</td>
<td>10</td>
<td>10±100</td>
</tr>
<tr>
<td>Iris</td>
<td>150</td>
<td>4</td>
<td>3</td>
<td>3±50</td>
</tr>
<tr>
<td>House Votes</td>
<td>232</td>
<td>16</td>
<td>2</td>
<td>124±104</td>
</tr>
<tr>
<td>Breast Cancer</td>
<td>683</td>
<td>9</td>
<td>2</td>
<td>444±239</td>
</tr>
</tbody>
</table>

(Sneath and Sokal, 1973) and complete-link (Sneath and Sokal, 1973) were applied for the unconstrained EAC, while the proposed constrained Average-link algorithm, a constrained version of single-link (Duarte et al., 2009) and a constrained version of complete-link (Klein et al., 2002) were used for the constrained EAC setting. The value of the softness parameter was set to \( p = 1 \). The number of clusters \( K^* \) of the consensus partitions was defined as the natural number of clusters \( K^0 \) for each data set. To build the sets of constraints using the RAC process and its variations, the size of the subset and the number of constraints was set to \( m = \lfloor 0.1n \rfloor \). For the RAL process and its variations, the size of the subset (i.e. the size of the labeled set) was set to \( m = \lfloor 0.1n \rfloor \). Each clustering combination method was applied 30 times for each data set.

To evaluate the performance of the combination methods we used the Consistency index (\( Ci \)) (Fred, 2001). \( Ci \) measures the fraction of shared data patterns in matching clusters of the consensus partition (\( P^* \)) and the real data partition (\( P^0 \)) obtained from ground-truth information. The Consistency index is computed as

\[
Ci(P^*, P^0) = \frac{1}{n} \min_{k} \frac{\sum_{C_i^* \cap C_i^0}}{\vert C_i^* \vert + \vert C_i^0 \vert}
\]

where it is assumed the clusters of \( P^* \) and \( P^0 \) have been permuted in a way that the cluster \( C_i^* \) matches with the real cluster \( C_i^0 \).

Table 2 presents the average Consistency index \( Ci(P^*, P^0) \times 100 \) values for the consensus partitions produced by the clustering combination methods using RAC process and variations. Column 1 shows the name of the data sets. Columns 2 to 4 (“Unconstrained”) presents the results for the unconstrained EAC using average-link (AL), single-link (SL) and complete-link (CL) algorithms. Columns 5 to 16 show the results of the constrained version of EAC using RAC, RAL and their variations for acquiring constraints, respectively, using constrained average-link (CAL), constrained single-link (CSL) and constrained complete-link (CCL) algorithms. It can be seen that the use of constraints usually (but not always) improves the quality of the consensus partitions. This is more evident when comparing the results produced by complete-link with the ones of constrained complete-link. The clustering algorithm used for extracting the consensus partition from the co-association matrix (AL, SL, CL, CAL, CSL and CCL) and constraint acquisition process (RAC, LRAC, HRAC, LHRAC, RAL, LRAL, HRAL and LHRA) with best performance was constrained average-link with LRAC, followed by con-
strained average-link again with LHRAC, achieving the best average CI results in 5 and 4 out of the 14 data sets, respectively. The complete-link and constrained complete-link algorithms never achieved the best result for any data set. These findings indicate that constrained average-link is a good constrained clustering algorithm for producing consensus partitions using the EAC framework, and that acquiring constraints in a subset of data patterns with low degree of confidence in their assignment to the clusters lead to an improvement of clustering quality.

Table 3 shows the results for the clustering combination methods using RAL process and variations. In fact, the unconstrained EAC never achieved a better result than the constrained EAC. The best combination of clustering algorithm and constraint acquisition process was constrained single-link with RAL, obtaining 8 best results out of 14 data sets, followed by constrained average with LRAL (again) which achieved 7 best results out of 14. The success of constrained single-link with RAL may be explained by the following facts: constrained single-link is a hard-constrained algorithm and the number of pairwise constraints obtained by using labels is very high and covers almost all the difficult cluster assignments in the data set. In this case, if the softness parameter of constrained average-link have been set to a higher value, probably its results should have been better. In fact, the combination of the constrained single-link algorithm with RAL process was the best for the synthetic data sets, obtaining the best results in 6 out of 7 data sets. Considering only the real data sets, the combination of the constrained average-link with LRAL process achieved the best results in 5 out of 7 real data sets. This supports the conclusion that using the constrained average-link algorithm for extracting the consensus partition, using the EAC framework, in conjunction with the LRAL process for acquiring constraints is a good choice for cluster real data sets. Once again, the best results were never produced by the complete-link and constrained complete-link algorithms.

By comparing the results from table 2 with the ones from table 3 we observe that the RAL process outperforms RAC. The advantage of using constraints in clustering combination is also more evident. This is due to the number of pairwise constraints acquired by RAL process being significantly higher than the number of constraints produced by RAC.

Table 4: Average Consistency index ($CI(P_i^*, P_i^{100})$) values for the consensus partitions produced by EAC, and Constrained EAC using RAL, LRAL, HRAL and LHRAL methods for acquirung constraints.

<table>
<thead>
<tr>
<th>Acquisition Method</th>
<th>Extractor Algorithm</th>
<th>Bars</th>
<th>Cites</th>
<th>D2</th>
<th>D3</th>
<th>Half Rings</th>
<th>Rings</th>
<th>Two Clusters</th>
<th>Wine</th>
<th>Std Yeast</th>
<th>Odpigists</th>
<th>Log Yeast</th>
<th>Iris</th>
<th>House Votes</th>
<th>Breast Cancer</th>
</tr>
</thead>
<tbody>
<tr>
<td>RAL</td>
<td>EAC</td>
<td>99.85</td>
<td>89.36</td>
<td>76.6</td>
<td>73.3</td>
<td>84.26</td>
<td>74.9</td>
<td>57.33</td>
<td>77.1</td>
<td>71.82</td>
<td>69.46</td>
<td>46.73</td>
<td>66.47</td>
<td>86.54</td>
<td>98.65</td>
</tr>
<tr>
<td>HRAL</td>
<td>EAC</td>
<td>99.85</td>
<td>89.36</td>
<td>76.6</td>
<td>73.3</td>
<td>84.26</td>
<td>74.9</td>
<td>57.33</td>
<td>77.1</td>
<td>71.82</td>
<td>69.46</td>
<td>46.73</td>
<td>66.47</td>
<td>86.54</td>
<td>98.65</td>
</tr>
<tr>
<td>LHRAL</td>
<td>EAC</td>
<td>99.85</td>
<td>89.36</td>
<td>76.6</td>
<td>73.3</td>
<td>84.26</td>
<td>74.9</td>
<td>57.33</td>
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<td>46.73</td>
<td>66.47</td>
<td>86.54</td>
<td>98.65</td>
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<tr>
<td>LHRAC</td>
<td>EAC</td>
<td>99.85</td>
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<td>76.6</td>
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<td>46.73</td>
<td>66.47</td>
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<td>98.65</td>
</tr>
</tbody>
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5 CONCLUSIONS AND FUTURE WORK

A new constrained agglomerative hierarchical clustering algorithm was proposed. It consisted in a modi-
fication to the average-link clustering algorithm. The soft-constrained average-link algorithm was applied in the EAC framework to produce the consensus partition using the co-association matrix as input and outperformed the hard-constrained clustering algorithms used for comparison.

The experimental results have shown that constrained clustering algorithms usually produce better consensus partitions than the traditional clustering algorithms, and that acquiring constraints from a subset of data containing the patterns with the lowest degree of confidence improves clustering quality.

Future work include the development of an “intelligent” algorithm for acquiring clustering constraints using the insights gained in this paper, the study of the effect of the softness parameter, and the establishment of criteria for its selection.

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