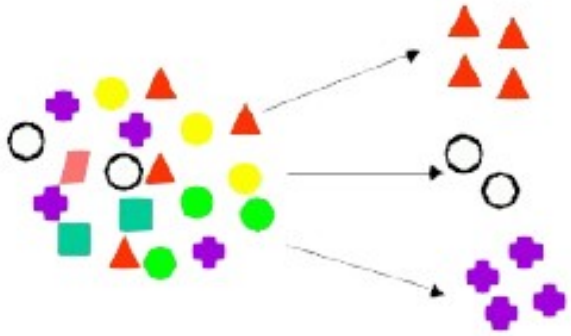

Efficient Evidence Accumulation Clustering for large datasets/big data

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Dedicated to someone special...

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Resumo

Avanços na tecnologia permitem a recolha e armazenamento de quantidades e variedades de dados sem precedente. A maior parte destes dados são armazenados eletrónicamente e existe interesse em realizar análise automática dos mesmos. As técnicas de *clustering* estão entre as mais populares para essa tarefa porque não assumem nada sobre a estrutura dos dados *a priori*. Dezenas de técnicas existem, mas, típicamente, uma só técnica não tem um bom desempenho em todos os conjuntos de dados devido às especifidades de cada um. Técnicas de *ensemble clustering* tentam responder a esse desafio ao combinar outros algoritmos. Esta dissertação foca-se numa em particular, o *Evidence Accumulation Clustering* (EAC). O EAC é uma algorithm robusto que tem demonstrado bons desempenhos na literatura numa variedade de conjuntos de dados. No entanto, esta robustez vem com um maior custo computacional associado. A sua aplicação não só é mais lenta como está restrita a conjuntos de dados pequenos. Assim, o objetivo desta dissertação é escalar o EAC, possibilitando a sua a aplicação a conjuntos de dados grandes (mais que $500\,000$ amostras), com tecnologia disponivel numa típica estação de trabalho. Com isto em mente, várias abordagens foram exploradas: acelerar processamento com outros algoritmos (*quantum clustering*), através de processamento paralelo (com GPU), escalar para maiores conjuntos de dados com algoritmos de memória externa (disco rígido) e explorando a natureza esparsa do EAC. Uma contribuição de relevo é um método novo para construir uma matriz de esparsa específico ao EAC. Os resultados mostram que a solução proposta é, efetivamente, aplicável a conjuntos de dados grandes e é significativamente mais rápida que a original para conjuntos pequenos.

Palavras-chave: clustering, EAC, quantum clustering, K-Means, Single-Link, matriz esparsa, GPGPU

Abstract

Advances in technology allow for the collection and storage of unprecedented amount and variety of data. Most of this data is stored electronically and there is an interest in automated analysis for generation of knowledge and new insights. Since, often, the structure of the data is unknown, clustering techniques become particularly interesting for knowledge discovery and data mining, since they makes as few assumptions on the data as possible. A vast body of work on these algorithms exist, yet, typically, no single algorithm is able to respond to the specificities of all data. Ensemble clustering algorithm address this problem by combining other algorithms. Evidence Accumulation Clustering (EAC) is a robust ensemble algorithm that has shown good results and is the focus of this dissertation. However, this robustness comes with higher computational cost. Its application is slower and restricted to smaller data sets. Thus, the objective of this dissertation is to scale EAC, allowing its applicability to big data sets (more than $500\ 000$ patterns), with technology available at a typical workstation. Accordingly, several approaches were explored: speed-up with other algorithms (*quantum clustering*) or parallel computing (with GPU) and reducing space complexity by using external memory (hard drive) algorithms and exploiting the sparse nature of EAC. A relevant contribution is a novel method to build a sparse matrix specialized in EAC. Results show that the proposed solution is applicable to large data sets and is significantly faster than the original for smaller data sets.

Key words: clustering, EAC, quantum clustering, K-Means, Single-Link, sparse matrix, GPGPU

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Glossary

API	Application Programming Interface.
CPU	Central Processing Unit.
EAC	Evidence Accumulation Clustering.
GPGPU	General Purpose computing in Graphics Processing Units.
GPU	Graphics Processing Unit.
HAC	Hierarchical Agglomeration Clustering.
PCA	Principal Component Analysis.
PC	Principal Component.
QK-Means	Quantum K-Means.
Qubit	Quantum bit.
SL-HAC	Single-Linkage Hierarchical Agglomeration Clustering.
SVD	Singular Value Decomposition.

Chapter 1

Clustering: basic concepts, definitions and algorithms

Hundreds of methods for data analysis exist. Many of these methods fall into the realm of machine learning, which is usually divided into 2 major groups: *supervised* and *unsupervised* learning. Supervised learning deals with labeled data, i.e. data for which ground truth is known, and tries to solve the problem of classification. Examples of supervised learning algorithms are Neural Networks, Decision Trees, Linear Regression and Support Vector Machines. Unsupervised learning deals with unlabeled data for which no extra information is known. An example of algorithms within this paradigm is clustering algorithms, which are the focus of this chapter.

This chapter will serve as an introduction to clustering. It starts by defining the problem of clustering in section 1.1, goes on to provide useful definitions and notation in section 1.2 and briefly addresses different properties of clustering algorithms in section 1.3. Two very well known algorithms are presented: K-Means in section 1.4 and Single-Link in section 1.5. Evidence Accumulation Clustering is a state of the art ensemble clustering algorithm and the focus of this dissertation. Section 1.6 will explain briefly the concept of ensemble clustering followed by an overview and application examples of the EAC algorithm in section 1.7.

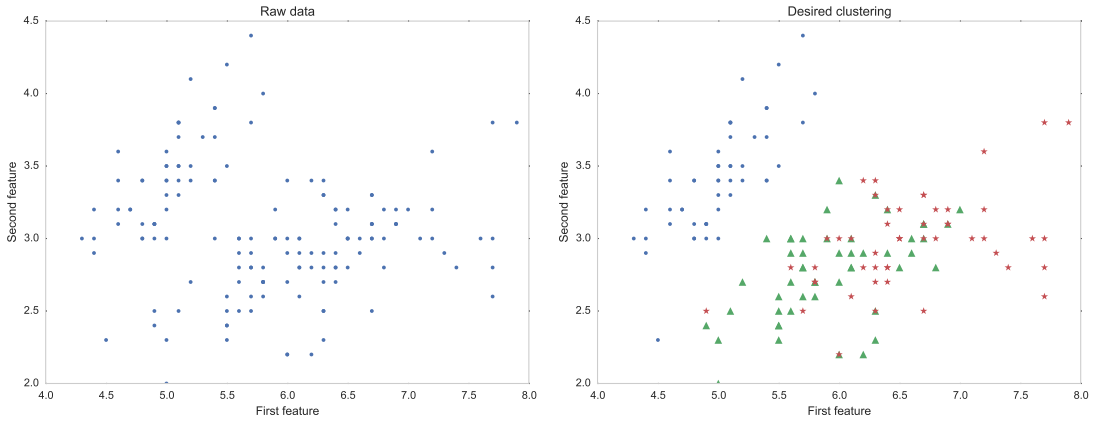
1.1 The problem of clustering

Cluster analysis methods are unsupervised and the backbone of the present work. The goal of data clustering, as defined by [1], is the discovery of the *natural grouping(s)* of a set of patterns, points or objects. In other words, the goal of data clustering is to discover structure on data. The methodology used is to group patterns (usually represented as a vector of measurements or a point in space [2]) based on some similarity, such that patterns belonging to the same cluster are typically more similar to each other than to patterns of other clusters. Clustering is a strictly data-driven method, in contrast with classification techniques which have a training set with the desired labels for a limited collection of patterns. Because there is very little information, as few assumptions as possible should be made

about the structure of the data (e.g. number of clusters). And, because clustering typically makes as few assumptions on the data as possible, it is appropriate to use it on exploratory structural analysis of the data. The process of clustering data has three main stages [2]:

- **Pattern representation** refers to the choice of representation of the input data in terms of size, scale and type of features. The input patterns may be fed directly to the algorithms or undergo *feature selection* and/or *feature extraction*. The former is simply the selection of which features of the originally available should be used. The latter deals with the transformation of the original features such that the resulting features will produce more accurate and insightful clusterings, e.g. Principal Component Analysis.
- **Pattern similarity** refers to the definition of a measure for computing the similarity between two patterns.
- **Grouping** refers to the algorithm that will perform the actual clustering on the dataset with the defined pattern representation, using the appropriate similarity measure.

As an example, Figure 1.1a shows the plot of the Iris data set [3, 4], a small well-known Machine Learning data set. This data set has 4 features, of which only 2 are represented, and 3 classes, of which 2 are overlapping. A class is overlapping another if they share part of the feature space, i.e. there is a zone in the feature space whose patterns might belong to either class. Figure 1.1b presents the desired clustering for this data set.



(a) Input data, unlabeled. (b) Desired labels.

Figure 1.1: First and second features of the Iris dataset. Fig. 1.1a shows the raw input data, i.e. how the algorithms ”see” the data. Fig. 1.1b shows the desired labels for each point, where each color is coded to a class.

1.2 Definitions and Notation

This section will introduce relevant definitions and notation within the clustering context that will be used throughout the rest of this document and were largely adopted from [2].

A *pattern* $\mathbf{x}$ is a single data item and, without loss of generality, can be represented as a vector of d *features* x_i that characterize that data item, $\mathbf{x} = (x_1, \ldots, x_d)$, where d is referred to as the dimensionality of the pattern. A *pattern set* (or data set) $\mathcal{X}$ is then the collection of all n patterns $\mathcal{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$. The number of features is usually the same for all patterns in a given pattern set.

In cluster analysis, the desired clustering, typically, is one that reflects the natural structure of the data, i.e. the original ground truth labeling. In other words, one wants to group the patterns that came from the same state of nature when they were generated, the same *class*. A class, then, can be viewed as a source of patterns and the effort of the clustering algorithm is to group patterns from the same source. Throughout this work, these classes will also be referred to as the "natural" or "true" clusterings. *Hard* clustering (or partitional) techniques assign a class label l_i to each pattern $\mathbf{x}_i$. The whole set of labels corresponding to a pattern set $\mathcal{X}$ is given by $\mathcal{L} = \{l_1, \ldots, l_n\}$, where l_i is the label of pattern $\mathbf{x}_i$. Closely related to the whole set of labels is the concept of a *partition*, which completely describes a clustering. A partition P is a collection of k *clusters*. A cluster C is a subset of nc patterns $\mathbf{x}_i$ taken from the pattern set, where the patterns belonging to one subset do not belong to any other in the same partition. A clustering *ensemble* $\mathbb{P}$ is a set N partitions P^j from a given pattern set, each of which is composed by a set of k_j clusters C_i^j, where $j = 1, \ldots, N$, $i = 1, \ldots, k_j$. Each cluster is composed by a set of nc_i^j patterns that does not intercept any other cluster of the same partition. The relationship between the above concepts is condensed in the following expressions:

$$\begin{aligned} ensemble \quad & \mathbb{P} = \left\{P^1, P^2, \ldots P^N\right\} \\ partition \quad & P^j = \left\{C_1^j, C_2^j, \ldots C_{k_j}^j\right\} \\ cluster \quad & C_i^j = \left\{x_1, x_2, \ldots x_{nc_i^j}\right\} \end{aligned}$$

Typically, a clustering algorithm will use a *proximity* measure for determining how alike are two patterns. A proximity measure can either be a *similarity* or a *dissimilarity* measure. One can easily be converted to the other and the main difference is that the former increases in value as patterns are more alike, while the latter decreases in value. A *distance* is a dissimilarity function *d* which yields non-negative real values and is also a *metric*, which means it obeys the following three properties:

$$\begin{aligned} identity \quad & d(\mathbf{x}_i, \mathbf{x}_i) = 0 \\ symmetry \quad & d(\mathbf{x}_i, \mathbf{x}_j) = d(\mathbf{x}_j, \mathbf{x}_i), i \neq j \\ triangle\ inequality \quad & d(\mathbf{x}_i, \mathbf{x}_j) + d(\mathbf{x}_j, \mathbf{x}_z) \geq d(\mathbf{x}_x, \mathbf{x}_z) \end{aligned}$$

where $\mathbf{x}_i$, $\mathbf{x}_j$ and $\mathbf{x}_z$ are 3 unique patterns belonging to the pattern set $\mathcal{X}$. Examples of proximity measures include the Euclidean distance, the Pearson's correlation coefficien and Mutual Shared Neighbors [5]. It should be noted that different proximity measures may be more appropriate in different contexts, such as document, biological or time-series clustering. Furthermore, data can come in different

types such as numerical (discrete or continuous) or categorical (binary or multinomial) attributes. The researcher should take these factors into account as different proximity measures are more appropriate for some type or even heterogeneous type data.

An introduction of clustering would be incomplete without a discussion on how good is a partition after clustering. Several *validation measures* exist and they can placed in two main categories [6]. *External* measures use *a priori* information about the data to evaluate the clustering against some external structure. An application of an external measure could be to test how accurate a clustering algorithm is for a particular dataset by matching the output partition against the ground truth. Examples of such measures include the *Consistency Index* [7] and the H-index [8]. *Internal* measures, on the other hand, determine the quality of the clustering without the use of external information about the data. The Davies-Bouldin index [9] is such a measure.

1.3 Characteristics of clustering techniques

Clustering algorithms may be categorized and described according to different properties. For the sake of completeness, a brief discussion of some of their properties will be layed out in this section.

It is common to organize cluster algorithms into two distinct types: *partitional* and *hierarchical*. A partitional algorithm, such as K-Means, is a hard clustering algorithm that will output a partiton where each pattern belongs exclusively to one cluster. A hierarchical algorithm produces a tree-based data structure called *dendrogram*. A dendrogram contains different partitions at different levels of the tree which means that the user can easily change the desired number of clusters by simply traversing the different levels. This is an advantage over a partitional algorithm since a user can analyze different partitions with different numbers of clusters without having to rerun the algorithm. Hierarchical algorithms can be further split into two approaches: bottom-up (or *agglomerative*) and top-down (or *divisive*). The former starts with all patterns as distinct clusters and will group them together according to some dissimilarity measure, building the dendrogram from the ground up; examples of algorithms that take this approach are Single-Link and Average-Link. The latter will start will all patterns in the same cluster and continuosly split it until all patterns are separated, building the dendrogram from the top level to the bottom; this approach is taken by the Principal Directon Divisive Partitioning[10] and Bisecting K-Means [11] algorithms.

Another characteristic relates to how algorithms use the features for computing similarities. If all features are used simultaniously the algorithm is called *polithetic*, e.g. K-Means. Otherwise, if the features are used sequentially, it is called *monothetic*, e.g. [12].

Contrasting *hard* clustering algorithm are the *fuzzy* algorithms. A fuzzy algorithm will attribute to each pattern a degree of membership to each cluster. A partition can still be extracted from this output by choosing, for each pattern, the cluster with higher degree of membership. An example of a fuzzy algorithm is the Fuzzy C-Means [13].

Another characteristic is an algorithm's stochasticity. A *stochastic* algorithms uses a probabilistic process at some point in the algorithms, possibly yielding different results in each run, e.g. K-Means

can use a random initialization. As an example, the K-Means algorithm typically picks the initialization centroids randomly. A *deterministic* algorithm, on the other hand, will always produce the same result for a given input, e.g. Single-Link.

Finally, the last characteristic discussed is how an algorithm processes the input data. An algorithm is said to be *incremental* if it processes the input incrementally, i.e. taking part of the data, processing it and then doing the same for the remaining parts, e.g. PEGASUS [14]. A *non-incremental* algorithm, on the other hand, will process the whole input in each run, e.g. K-Means. This discussion is specially relevant when considering large datasets that may not fit in memory or whose processing would take too long for a single run and is therefore done in parallel.

1.4 K-Means

One of the most famous non-optimal solutions for the problem of partitional clustering is the K-Means algorithm [15]. The K-Means algorithm uses K *centroid* representatives, c_k, for K clusters. Patterns are assigned to a cluster such that the squared error (or, more accurately, squared dissimilarity measure) between the cluster representatives and the patterns is minimized. In essence, K-Means is a solution (although not necessarily an optimal one) to an optimization problem having the Sum of Squared Errors as its objective function, which is known to be a computationally NP hard problem [1]. It can be mathematically demonstrated that the optimal representatives for the clusters are the means of the patterns of each cluster [6]. K-Means, then, minimizes the following expression, where the proximity measure used is the Euclidean distance:

$$\sum_{k=1}^{K} \sum_{\mathbf{x}_i \in C_k} \|\mathbf{x}_i - c_k\|^2 \tag{1.1}$$

K-Means needs two initialization parameters: the number of clusters and the centroid initializations. It starts by assigning each pattern to its closer cluster based on the cluster's centroid. This is called the **labeling** step since one usually uses cluster labels for this assignment. The centroids are then recomputed based on this assignment, in the **update** step. The new centroids are the mean of all the patterns belonging to the clusters, hence the name of the algorithm. These two steps are executed iteratively until a stopping condition is met, usually the number of iterations, a convergence criteria or both. The initial centroids are usually chosen randomly, but other schemes exist to improve the overall accuracy of the algorithm, e.g. K-Means++ [16]. There are also methods to automatically choose the number of clusters [6].

The proximity measure used is typically the Euclidean distance. This tends to produce hyperspherical clusters [2]. Still, according to [1], other measures have been used such as the L1 norm, Mahalanobis distance, as well as the cosine similarity [6]. The choice of similarity measure must be made carefully as it may not guarantee that the algorithm will converge.

A detail of implementation is what to do with clusters that have no patterns assigned to them. One

approach to this situation is to drop the empty clusters in further iterations. However, allowing the existence of empty clusters or dropping empty clusters is undesirable since the number of clusters is an input parameter and it is expected that the output contains the specified number of clusters. Other approaches exist dealing with this problem, such as equaling the centroid of an empty cluster to the pattern furthest away from its assigned centroid or reusing the old centroids as in [17].

K-Means is a simple algorithm with reduced complexity $O(ntk)$, where n is the number of patterns in the pattern set, k is the number of clusters and t is the number of iterations that it executes. Accordingly, K-Means is often used as foundational step of more complex and robust algorithms, such as the EAC algorithm.

As an example, the evolution and output of the K-means algorithm to the data presented in Fig. 1.1 is represented in Fig. 1.2. The algorithm was executed with 3 random centroids.

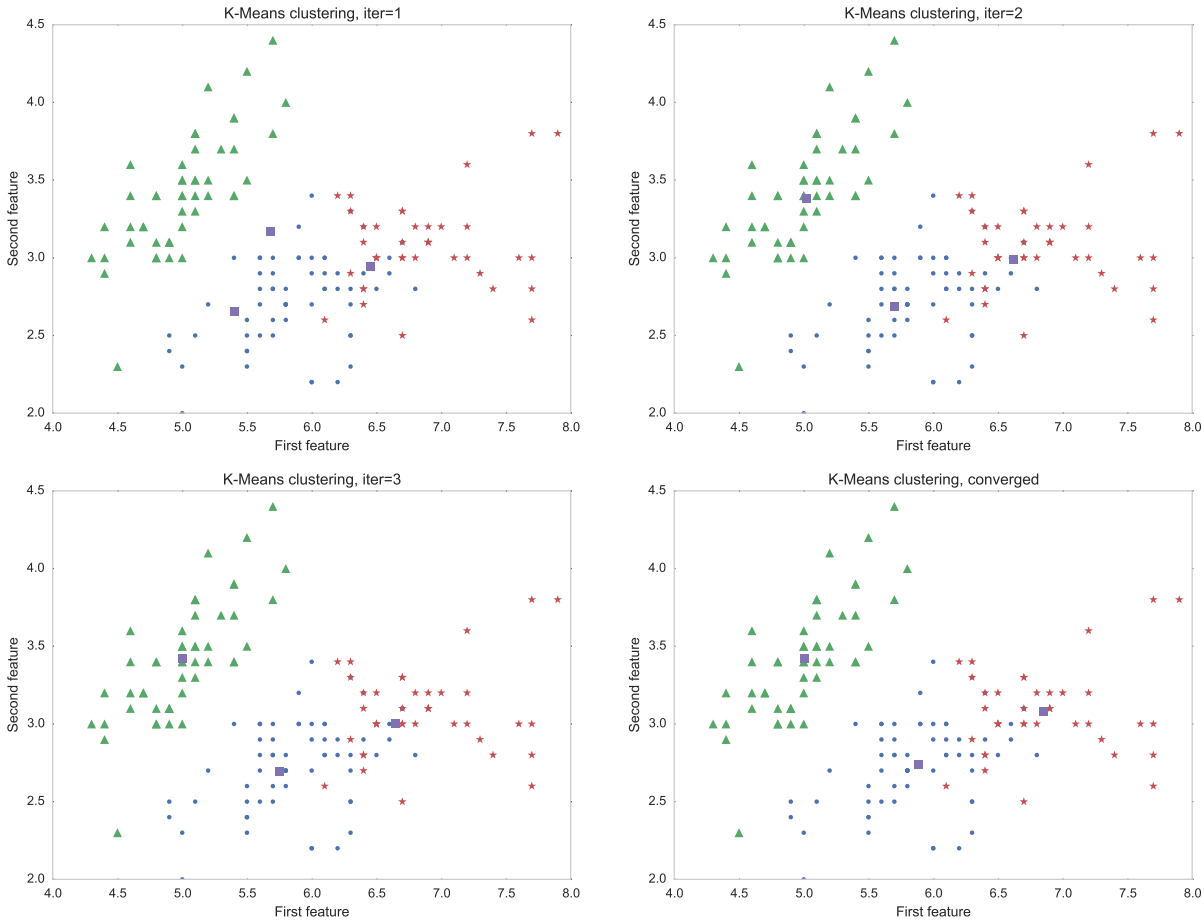


Figure 1.2: The output labels of the K-Means algorithm with the number of clusters (input parameter) set to 3. The different plots show the centroids (squares) evolution on each iteration. Between iteration 3 and the converged state 2 more iterations were executed.

Even with the correct number of clusters, the clustering results do not match 100% the natural clusters. The accuracy relative to the natural clusters of Fig. 1.1b is 88% as measured by the Consistency Index (CI) [7]. In this example, the problem is the two overlapping clusters. It is hard for an algorithm to discriminate between two clusters when they have similar patterns. When no prior information about the dataset is given, the number of clusters can be hard to discover. This is why, when available, a domain

expert may provide valuable insight on tuning the initialization parameters.

1.5 Single-Link

Single-Link [18] is one of the most popular hierarchical agglomerative clustering (HAC) algorithms. HAC algorithms operate over a pair-wise dissimilarity matrix and outputs a dendrogram (e.g. Fig 1.4a). The main steps of an agglomerative hierarchical clustering algorithm are the following [2]:

1. Create a pair-wise dissimilarity matrix of all patterns, where each pattern is a distinct cluster singleton;

2. Find the closest clusters, merge them and update the matrix to reflect this change. The rows and columns of the two merged clusters are deleted and a new row and column are created to store the new cluster.

3. Stop if all patterns belong to a single cluster, otherwise continue to step 2.

The algorithm stops when $n-1$ merges have been performed, which is when all patterns have been connected in the same cluster. Just like in the K-Means algorithm, different similarity measures can be used for the distances.

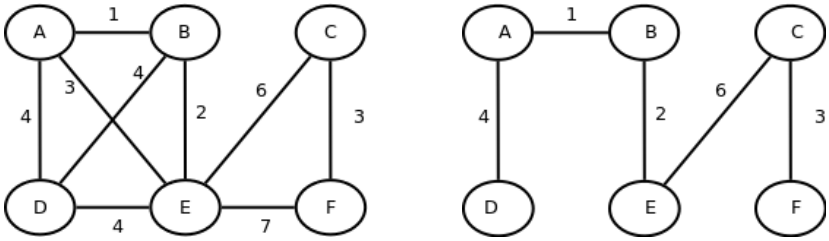
The proximity between clusters in the second step is distinguishes between the different HAC linkage algorithms, such as Single-Link , Average-Link, Complete-Link, among others. In Single-Link (SL), the proximity between any two clusters is the the dissimilarity between their closest patterns. On the other hand, in Complete-Link, it is the proximity between their most distant patterns and, in Average-Link, is the proximity between the average point of each cluster. In SL, because the algorithm connects first clusters that are more similar, it naturally gives more importance to regions of higher density [6].

The total time complexity of a naive implementation is $O(n^3)$ since it performs a $O(n^2)$ search in step two and it does it $n-1$ times. Over time, more efficient implementations have been proposed, such as SLINK [19]. SLINK needs no working copy of $O(n^2)$ the pair-wise similarity matrix (if the original can be modified), has a working memory of $O(n^2)$ and time complexity of $O(n^2)$. This increase in performance comes from the observation that the $O(n^2)$ search can be transformed in a $O(n)$ search at the expense of keeping two arrays of length n that will store the most similar cluster for each pattern and the corresponding similarity measure. This way, to find the two closest clusters, the algorithm will not search the entire similarity matrix, but only the new similarity array since this array keeps the closest cluster of each cluster. Naturally these arrays must be updated upon a cluster merge.

An interesting property of the SL algorithm is its equivalence with a Minimum Spanning Tree (MST), an observation first made by [20]. In graph theory, a MST is a tree that connects all vertices together while minimizing the sum of all the distance between them. An example of a graph and its corresponding MST can be seen in Fig. 1.3. In this context, the edges of the MST are the distances between the patterns and the vertices are the patterns themselves. A MST contains all the information necessary to build a Single-Link dendrogram. To walk down through the levels of the dendrogram from the MST, one

cuts the least similar edges. Furthermore, this approach can be used to apply Single-Link clustering to graphs-encoded problems in a straight-forward way. Furthermore, the performance properties of this method are roughly the same as SLINK [21].

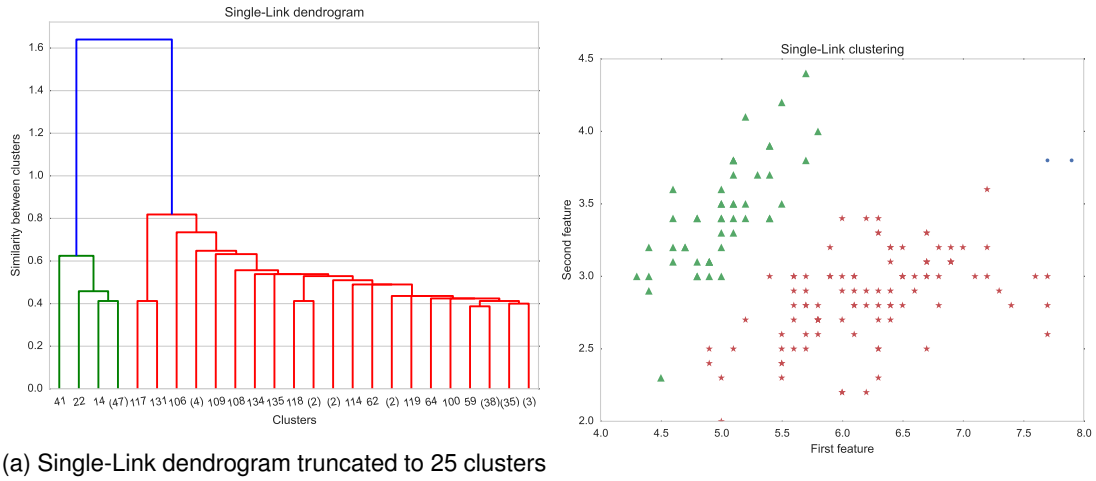
The true advantage of using an MST based approach comes when the number of edges (similarities) m of the MST is less than $\frac{n(n-1)}{2}$, where n is the number of nodes (patterns) [22]. This is because SLINK works over a inter pattern similarity matrix, meaning that the similarity between every pair of patterns must be explicitly represented. The minimum number of similarities is $\frac{n(n-1)}{2}$, which is equivalent to the upper or lower half triangular matrices of the similarity matrix. The MST, on the other hand, works over a graph that may or may not have edges between every pair of nodes. Fast MST algorithms have a time complexity of $O(mlogn)$, which is an improvement over $O(n^2)$ when $m << \frac{n(n-1)}{2}$.



(a) Example of a graph. (b) MST of the graph to the left.

Figure 1.3: The above figures show an example of a graph (left) and its corresponding Minimum Spanning Tree (right). The circles are vertices and the edges are the lines linking the vertices.

An example of a Single-Link dendrogram and resulting cluster can be observed in Fig. 1.4. The dendrogram in Fig. 1.4a has been truncated to 25 clusters in the bottom level for the sake of readability. The clustering presented on Fig. 1.4b is the result of cutting the dendrogram such that only 3 clusters exist (the number of classes). The accuracy, as measured by the CI, is of 58%.



(a) Single-Link dendrogram truncated to 25 clusters in the bottom level.

(b) Clustering with 3 clusters.

Figure 1.4: The above plots show the dendrogram and a possible clustering taken from a Single-Link run over the Iris data set. Fig. 1.4b was obtained by performing a cut on a level that would yield a partition of 3 clusters.

1.6 Ensemble Clustering

The underlying idea behind ensemble clustering is to take a collection of partitions, a *clustering ensemble*, and combine it into a single partition. There are several motivations for ensemble clustering. Data from real world problems appear in different configurations regarding shape, cardinality, dimensionality, sparsity, etc. Different clustering algorithms are appropriate for different data configurations, e.g. K-Means tends to group patterns in hyperspheres [2] so it is more appropriate for data whose structure is formed by hypershere like clusters. If the true structure of the data at hand is heterogeneous in its configuration, a single clustering algorithm might perform well for some part of the data while other performs better for some other part. Since different algorithms can be used to produce the partitions in the ensemble, one can use a mix of algorithms to address different properties of the data such that the combination is more **robust** to noise and outliers [23] and the final clustering has a **better quality** [6]. Ensemble clustering can also be particularly useful in situations where one does not have direct access to all the features of a given data set but can have access to partitions from different subsets and later combining with an ensemble algorithm. Furthermore, the generation of the clustering ensemble can be **parallelized and distributed** since each partition is independent from every other partition.

A clustering ensemble, according to [24], can be produced from (1) different data representations, e.g. choice of preprocessing, feature selection and extraction, sampling; or (2) different partitions of the data, e.g. output of different algorithms, varying the initialization parameters on the same algorithm.

Ensemble clustering algorithms can take three main distinct approaches [6]: based on pair-wise similarities, probabilistic or direct. EAC [24] and CSPA [25] are examples of pair-wise similarity based approach, where the algorithms use a co-associations matrix. The MMCE [23] and BCE [26] are examples of a probabilistic approach. This approach will be further clarified when the EAC algorithm is explained. HGPA [25], MCLA [25] and bagging [27] are examples of a direct approach to combining the ensemble clusterings, where the algorithms work directly with the labels without creating a co-association matrix. A detailed and thorough review of the similarity measures that can be used on with clustering ensembles and the state of the art algorithms can be consulted in [6].

1.7 Evidence Accumulation Clustering

1.7.1 Overview

The goal of EAC is to find an optimal partition P^* containing k^* clusters, from the clustering ensemble $\mathbb{P}$. The optimal partition should have the following properties [24]:

- **Consistency** with the clustering ensemble;
- **Robustness** to small variations in the ensemble; and,
- **Goodness** of fit with ground truth information, when available.

Ground truth is the true labels of each sample of the dataset, when such exists, and is used for validation purposes. Since EAC is an unsupervised method, this typically will not be available. EAC makes no assumption on the number of clusters in each data partition. Its approach is divided in 3 steps:

1. **Production** of a clustering ensemble $\mathbb{P}$ (the evidence);
2. **Combination** of the ensemble into a co-association matrix;
3. **Recovery** of the natural clusters of the data.

In the first step, a clustering ensemble is produced. Within the context of EAC, it is of interest to have variety in the ensemble with the intention to better capture the underlying structure of the data. One such parameter to measure that variety is the number of clusters in the partitions of the ensemble. Typically, the number of clusters in each partition is drawn from an interval $[K_{min}, K_{max}]$ with uniform probability. This influences other properties of other parts of the algorithm such as the sparsity of the co-association matrix as will become clearer in future chapters. Reviewing the literature [28, 24, 29, 30], it is clear the ensemble is usually produced by random initialization of K-Means (specifying only the number of centroids within the above interval). Still, other clustering algorithms have been used for the production of the ensemble [31] such as Single-Link, Average-Link and CLARANS.

The ensemble of partitions is combined in the second step, where a non-linear transformation turns the ensemble into a co-association matrix [24], i.e. a matrix $\mathcal{C}$ where each of its elements n_{ij} is the association value between the pattern pair (i, j). The association between any pair of patterns is given by the number of times those two patterns appear clustered together in any cluster of any partition of the ensemble, i.e. the number of co-occurrences in the same cluster. The rationale is that pairs that are frequently clustered together are more likely to be representative of a true link between the patterns [28], revealing the underlying structure of the data. In other words, a high association n_{ij} means it is more likely that patterns i and j belong to the same class. The construction of the co-association matrix is at the very core of this method.

The co-association matrix itself is not the output of EAC. Instead, it is used as input to other methods to obtain the final partition. The co-association between any two patterns can be interpreted as a similarity measure. Thus, since this matrix is a similarity matrix it's appropriate to use algorithms that take this type of matrices as input, e.g. K-Medoids or hierarchical algorithms such as Single-Link or Average-Link, to name a few. Typically, algorithms use a distance as the dissimilarity, which means that they minimize the distance to obtain the highest similarity between objects. However, a low value on the co-association matrix translates in a low similarity between a pair of objects, which means that the co-association matrix requires prior transformation for accurate clustering results, e.g. replace every similarity value n_{ij} between every pair of object (i, j) by $max\{\mathcal{C}\} - n_{ij}$.

Although any algorithm can be used, the final clustering is usually done using SL or AL. Each of this algorithms will take as input the transformed co-association matrix as the dissimilarity matrix. Furthermore, not knowing the "natural" number of clusters one can use the lifetime criteria, i.e. the number of

clusters k should be such that it maximizes the cost of cutting the dendrogram from $k-1$ clusters to k. Further details on the lifetime strategy for picking the number of clusters falls outside the scope of this work and are presented in [24].

Related work to EAC has been developed. The Weighted EAC (WEAC) algorithm [31] and a study on the sparsity of the co-association matrix [32] should be mentioned. The latter is discussed in more depth in chapter **??**. The former introduces the novelty of having weights associated to each partition such that good quality partitions are more relevant than their counterparts. These weights are based on internal validity measures. Weighing the partitions in terms of quality has shown to improve the original algorithm, accuracy wise.

1.7.2 Examples of applications

EAC has been used with success in several areas. Some of its applications are:

- in the field of bioinformatics it was used for the automatic identification of chronic lymphocyt leukemia [33];
- also in bioinformatics it was used for the unsupervised analysis of ECG-based biometric database to highlight natural groups and gain further insight [30];
- in computer vision it was used as a solution to the problem of clustering of contour images (from hardware tools) [29].

Chapter 2

Results and Discussion

The present chapter is dedicated to the results relevant to the work produced and their associated interpretation and subsequent discussion.

2.1 EAC

This section will present thorough results concerning several characteristics related to the EAC method. These were the timings of the different parts, how cardinality and the different K_{min} rules affected the sparsity of the co-association matrix, the typical number of associations per cluster in each rule, the growth of the number of associations with the different parameters, among others. Two mixture of Gaussians of 6 clusters, 10 million patterns and two dimensions were generated. A variation of the number of dimensions has more interest in the production phase. Since the production of the ensemble uses K-Means, detailed results can be found in section **??**. One mixture has overlapping Gaussians and the other does not. The reasoning was that overlapping Gaussians might result in more associations per cluster.

Throughout this section, different rules for computing the K_{min} and different co-association matrix formats will be mentioned. The different formats for the co-association matrix have been presented in chapter **??**. The different rules and their aliases are presented in Table 2.1.

Table 2.1: Different rules for computing K_{min} and K_{max}. n is the number of patterns in the data set and sk is the number of samples per cluster.

Rule	K_{min}	K_{max}
sqrt	$\frac{\sqrt{n}}{2}$	$\sqrt{n}$
2sqrt	$\sqrt{n}$	$2\sqrt{n}$
sk=sqrt2	$sk = \frac{\sqrt{n}}{2}$	$1.3K_{min}$
sk=300	$sk = 300$	$1.3K_{min}$

The experiment that generated the results of these section was set up as follows. A large data set was generated. The data set was sampled uniformly to produce a smaller data set with the desired number of patterns. A clustering ensemble was produced (production phase) for each of these smaller

data sets and for each of the rules, using K-Means. From each ensemble, co-association matrices of every applicable format were built (combination phase). A matrix format was not applicable when the data set complexity would make its correspondent co-association matrix too big to fit in main memory. The final clustering (recovery phase) was also done for each of the matrix formats. SLINK was used with fully allocated formats and the MST-based SL (SL-MST) and MST-based SL on external memory (SL-MST-disk) were executed with sparse matrices. SL-MST was not executed if its space complexity was too big to fit in main memory. Furthermore, the combination and recovery phases were repeated several times for smaller data sets for statistical relevant of the execution times, so as to make the influence of any background process less salient. For big data sets, the execution times are big enough that the influence of background processes is negligible.

2.1.1 Building the co-association matrix

The execution times for the combination phase can be observed in Figures 2.2 and 2.3, which allow the comparison between the different rules and the different matrix formats, respectively. To avoid redundancy, only one matrix format is depicted to compare the execution times for the different rules and only one rule to compare the matrix formats. The results of the other cases follow the same pattern. These times are related with the K_{min} parameter, whose evolution is presented in Fig. 2.1. Rules *sqrt*, *2sqrt* and *sk=sqrt2* never intersect but rule $sk = 300$ intersects all of them. Observing Fig. 2.2, one can see that the same thing happens to the execution time associated with the $sk = 300$ rule. A higher K_{min} means more centroids for each K-Means run to compute, so it is not surprising that, has K_{min} increases the execution time for computing the ensemble also increases.

In a previous section, the execution times for the combination phase had already been briefly presented when comparing different sparse formats. Fig. 2.3 shows the execution times on a longitudinal study for optimized matrix formats. It is clear that the sparse formats are significantly slower than the fully allocated ones, specially for smaller data sets. The *full condensed* format usually takes close to half the time than the *full* format, which is natural given that it performs half the operations. Idem for the *sparse condensed* formats compared to the *sparse complete*. The big discrepancy between the sparse and full formats is that the former needs to do a binary search at each association update and needs to keep the internal sparse data structure sorted.

2.1.2 SLINK vs SL-MST vs SL-MST-Disk

The clustering times of the different methods of SL discussed previously (SLINK, SL-MST and SL-MST-Disk) are presented in Figures 2.4, 2.5 and 2.6. The SL-MST-Disk method is significantly slower than any of the other methods. This is expected, since it uses the hard drive which has very slow access times compared to main memory. SL-MST is faster than SLINK, since it processes zero associations while SL-MST takes advantage of a graph representation and only processes the non-zero associations. In resemblance to what happened with combination times, the condensed variants take roughly half the time has their complete counterparts. This is expected, since SL-MST and SL-MST-Disk over condensed

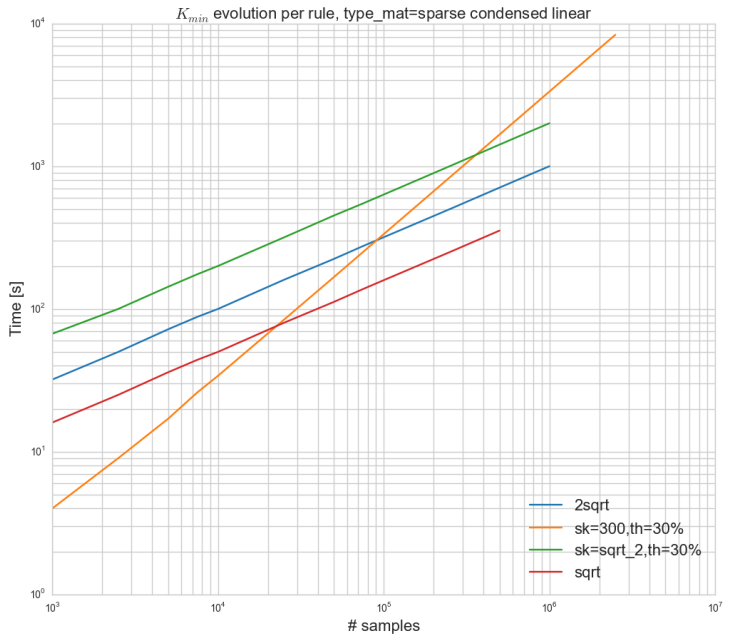


Figure 2.1: Evolution of K_{min} with cardinality for different rules.

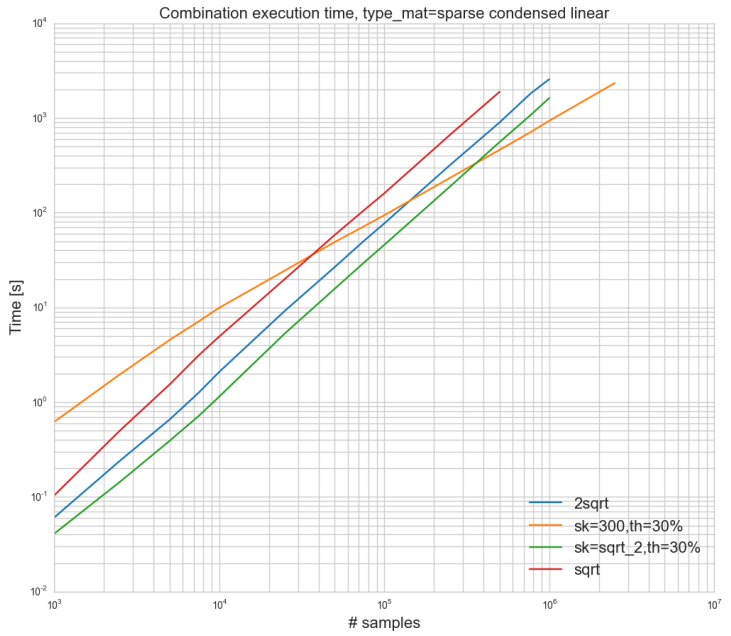


Figure 2.2: Execution time for building the co-association matrix from ensemble with different rules.

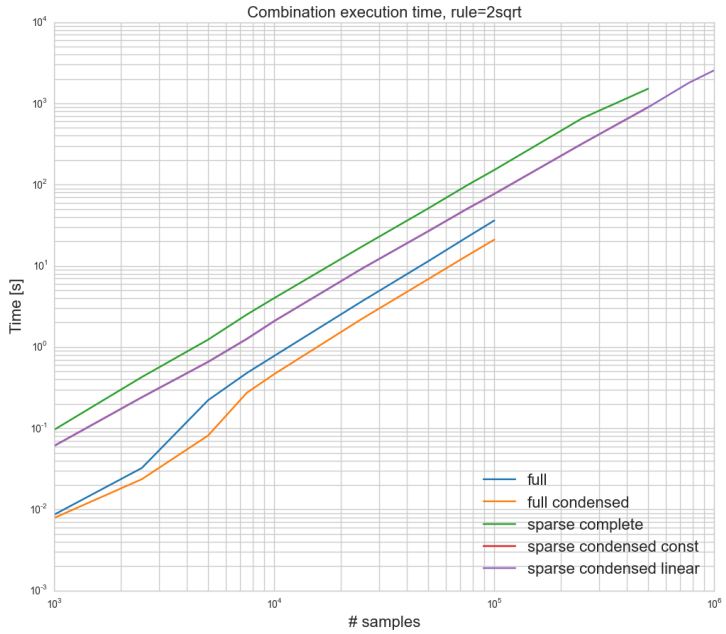


Figure 2.3: Execution time for building the co-association matrix with different matrix formats.

co-association matrices only process half the number of associations. SLINK takes roughly the same time for every rule, which means K_{min} has no influence, since SLINK processes both zero and non-zero associations and K_{min} only influences the number of non-zero associations. The same rationale can be applied to SL-MST, where different rules can have significant influence over execution time, since they change the total number of associations. As with the combination phase, the execution time referent to the *sk=300* rule started with the greatest time and decreased with an increase in cardinality until it was the fastest.

2.1.3 Analysis of the number of associations

The sparse nature of EAC has been referred to before and is clearer in Fig. 2.7. This figure shows the association density, i.e. number of associations relative to the n^2 associations in a full matrix. The *full condensed* format as a constant density of 49.5% and the density of *sparse complete* is two times that of the *sparse condensed* formats. The overall tendency is for the density to decrease as the number of patterns of the data set increases. This is to be expected since the *full* matrix grows quadratically. Besides, it would be expected that the same associations would be grouped together more frequently in partitions and simply previous connections stronger instead of creating new ones. Results presented in Fig. 2.9, which presents the number of associations per pattern, suggest otherwise. The number of associations per pattern increases with the number of patterns of the data set, with the notable exception of the *sk=300* rule which increases until it reaches a certain limit and then stabilizes. This is explained by the fact that this rule is based on setting a maximum constant number (300) of patterns in any given cluster, while in the other rules this number increases with the number of patterns. The number of patterns per pattern is not 300 for the $sk = 300$ rule because a pattern will be clustered with different neighbors in different partitions. Still, the number of neighbors doesn't change enough that the

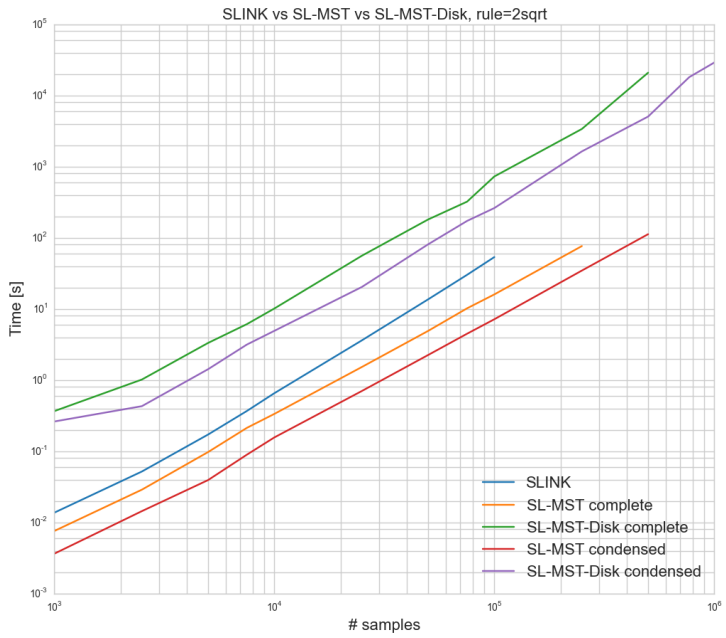


Figure 2.4: Comparison between the execution times of the three methods of SL. SLINK runs over fully allocated condensed matrix while SL-MST and SL-MST-Disk run over the condensed and complete sparse matrices.

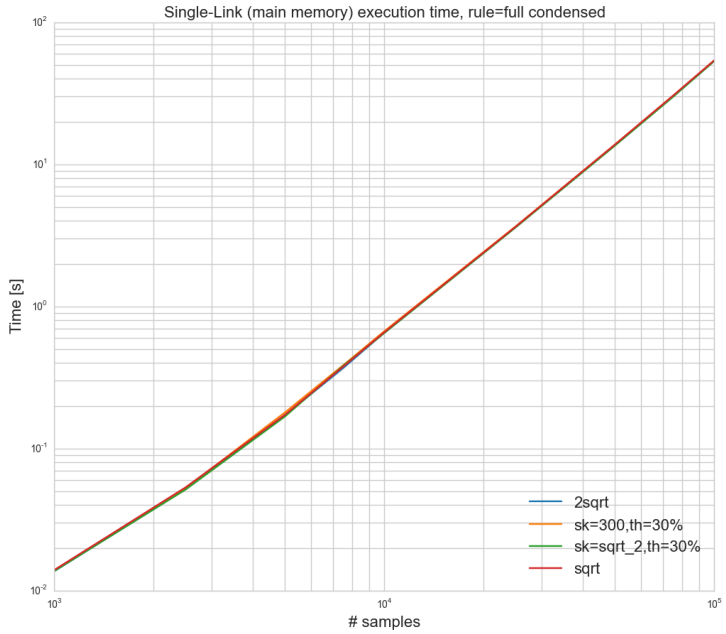


Figure 2.5: Comparison between the execution times of SLINK to different rules.

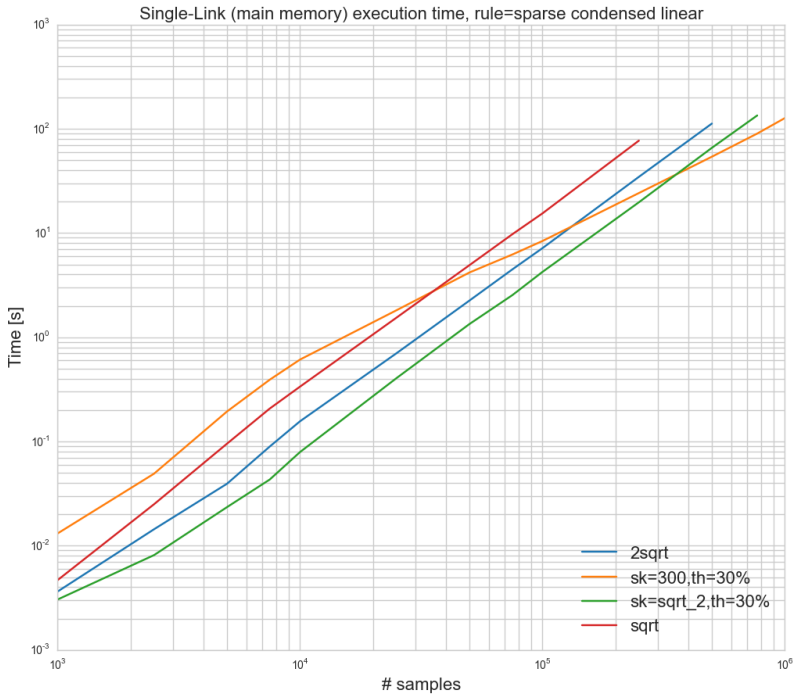


Figure 2.6: Comparison between the execution times of the three methods of SL over condensed matrices. SLINK runs over fully allocated condensed matrix while SL-MST and SL-MST-Disk run over the sparse matrix.

number of associations per pattern increases boundlessly. In fact, Fig. 2.9 suggests that the number of associations per pattern is around 3 times the upper bound on the number of patterns per cluster (strictly related to K_{min}). So, the decrease in density is more related with the quadratic growth of the *full* matrix in contrast with a linear growth of the number of associations.

Predicting the number of associations before building the co-association matrix is useful for coming up with combination schemes that are both memory and speed efficient. It was stated before that the biggest cluster size in any partition of the ensemble is a good parameter for this end. Fig. 2.9 presents the relationship between the biggest cluster size and the maximum number of associations of any pattern. These ratio increases with the number of patterns in the beginning, but as the number of patterns increases it never goes over 3, which further reinforces the previous statement.

The dimensionality of the used data sets is rather reduced. One would expect that this ratio would increase with the number of dimensions, since there would be more degrees where the clusters might include other neighbors. With this in mind, further studies ranging a wider spectrum of data sets should yield more enlightening conclusions or reinforce those presented here.

2.1.4 Space complexity

The previous section analyzed results related to the number of associations. This is related to the space complexity of the different matrix formats, but does not present an accurate depiction of their complexity.

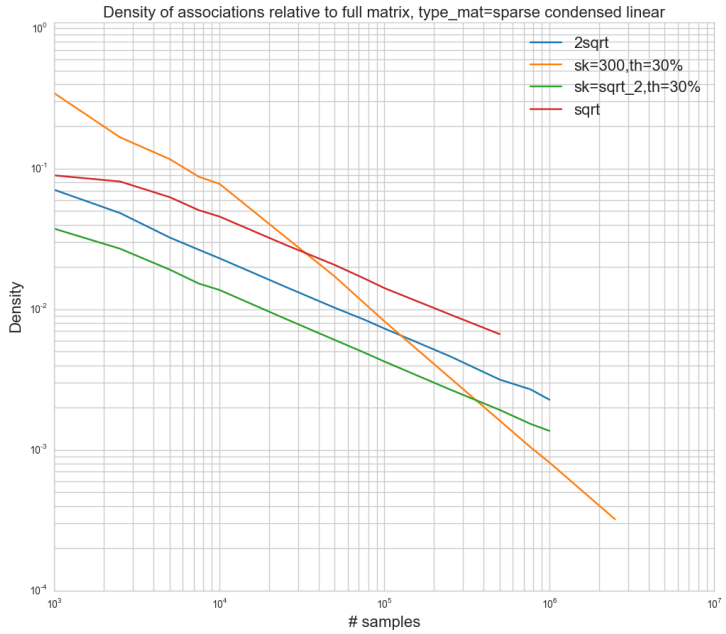


Figure 2.7: Density of associations relative to the full co-association matrix, which hold n^2 associations.

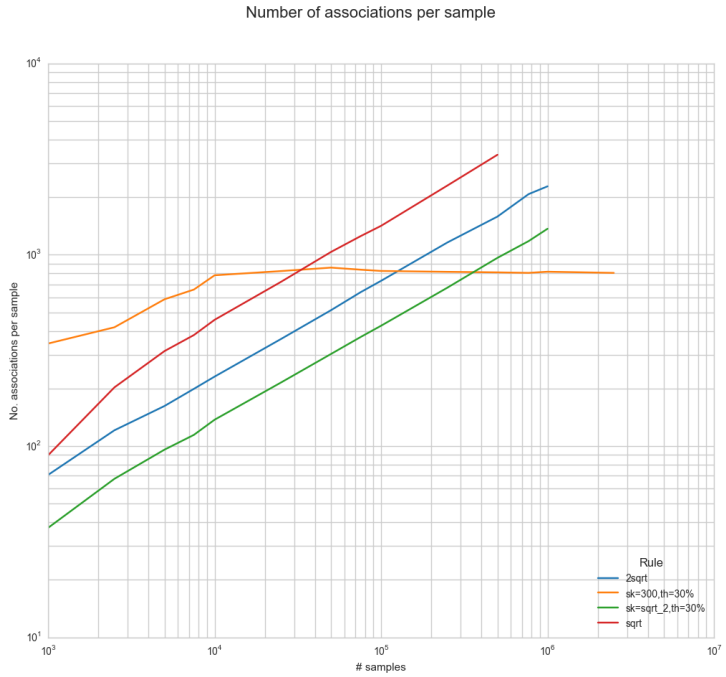


Figure 2.8: Evolution of the total number of associations divided by the number of patterns according to the different rules.

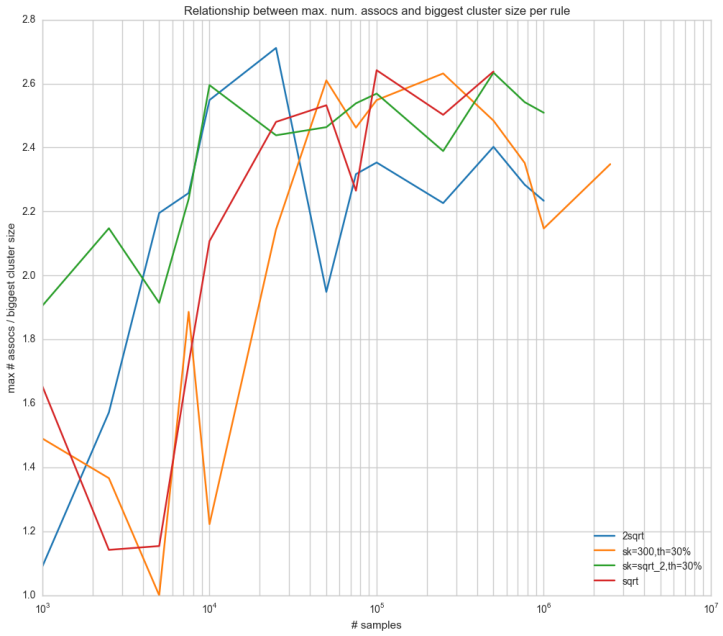


Figure 2.9: Maximum number of associations of any pattern divided by the number of patterns in the biggest cluster of the ensemble.

Chapter 3

Discussion?

3.1 real num assocs compared to samples per cluster

[32] reports that, on average, ẗhe overall contribution of the clustering ensemble (including unbalanced clusters) duplicates the co-associations produced in a single balanced clustering with Kmin clusters.̈ However, the spectrum of datasets evaluated regarding cardinality was smaller than that evaluated in the present work. The results suggest that the contribution of the ensemble is in fact higher.

3.2 Trade-off speed accuracy memory

When a problem of clustering of big data is at hand, the user should reflect upon what the problem at hand really requires: speed or accuracy. The user should take into consideration the nature of the data and the requirements of the problem (concerning speed and accuracy) before proceeding to the execution of the analysis. The present body of work reflects a method of clustering over big data using a high accuracy, but also high cost, method. Other methods offer the opposite, low cost, low to average accuracy.

3.3 Expanding this work to other scalability paradigms

The present work focused on two main approaches for scalability: GPGPU and out-of-core solution. A current trend in computing of big data is cluster computing, which allows for distributed and parallel computing. For the sake of completeness it is interesting to discuss if the ideas related to the former two paradigms are transferable to the later.

The concept of GPGPU is one of parallelization. It is based on the fact that each computing thread in the GPU will execute instructions on a restricted subset of the entire dataset. This idea is easily transferable to cluster computing, as it is a core concept on both paradigms. For this reason, the generation of the ensemble is a step of EAC that can be very easily transfered to a computing cluster.

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