HSC: A Novel Method for Clustering Hierarchies of Networked Data

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“Scientific knowledge is organized in levels, not because reduction in principle is impossible, but because nature is organized in levels, and the pattern at each level is most clearly discerned by abstracting from the detail of the levels far below.”

H. A. Simon
Abstract

Hierarchical clustering is one of the most powerful solutions to the problem of clustering, on the grounds that it performs a multi scale organization of the data. In recent years, research on hierarchical clustering methods has attracted considerable interest due to the demanding modern application domains.

We present a novel divisive hierarchical clustering framework called Hierarchical Stochastic Clustering (HSC), that acts in two stages. In the first stage, it finds a primary hierarchy of clustering partitions in a dataset. In the second stage, feeds a clustering algorithm with each one of the clusters of the very detailed partition, in order to settle the final result. The output is a hierarchy of clusters. Our method is based on the previous research of Meyer and Weissel Stochastic Data Clustering and the theory of Simon and Ando on Variable Aggregation.

Our experiments show that our framework builds a meaningful hierarchy of clusters and benefits consistently the clustering algorithm that acts in the second stage, not only computationally but also in terms of cluster quality. This result suggest that HSC framework is ideal for obtaining hierarchical solutions of large volumes of data.
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Chapter 1

Introduction

Clustering analysis, as one of the widely-adopted key tools in handling statistical data, is ubiquitous in many fields of data analysis such as bioinformatics, machine learning, data mining and many more [1]. In recent years, research on clustering methods has attracted considerable interest due to the demanding modern application domains along with the transition to the era of big data. The term big data describes unstructured data produced and stored in large volumes and different varieties. Those changes created the need for more efficient clustering methods, that aim to connect and correlate relationships, hierarchies and multiple data linkages and find hidden structures in the data. This approach can lead to more efficient processing, interpretation and visualization. From the machine learning perspective, clusters correspond to hidden structures or patterns and their extraction can be done an unsupervised way.

1.1 Hierarchical Clustering

Clustering is the task of organizing a set of data items into groups with respect to their features, in a way that the items that belong to the same cluster have a higher similarity than those of different clusters. Clustering methods can be classified in categories such as partitioning, grid-based, constraint-based and more [7, 58]. In this work, we consider that hierarchical clustering as a powerful solution to the problem, on the grounds that it performs a multi scale organization of the data and thus it results in more qualitative clustering. The central role of hierarchical clustering in data mining was stressed by several studies which have gained considerable attention from the community [40, 62].

According to Simon [52, 56], real and artificial-world complex systems are often hierarchically organized, in other words, they tend to be structured in layers of
levels. This fundamental property is called *near-decomposability*, and will be discussed in detail subsequently in this thesis. Later studies [10, 49, 34, 22] confirm the observation. According to them, hierarchical clustering can be applied in networks, such as protein interaction networks, metabolic networks, brain networks and is capable of offering insight into many network phenomena. Moreover, apart from networks, hierarchical clustering has applications in other domains and high-dimensional real-world arising data [15], with the text clustering being one of most representative examples [59].

Hierarchical clustering builds a cluster tree, most commonly named as *dendrogram*, where every cluster node contains child clusters. In this way, clusters can be viewed as ordered sets organized according to a relationship, both among themselves and within the whole. Relationships vary according to the field domain and type of system, but generally, they can be described by a similarity or dissimilarity (distance) measure.

As it is known, there is no shortage of hierarchical clustering algorithms in literature. Hierarchical clustering solutions have been primarily obtained using *agglomerative* (bottom-up) schemes, such as *Birch* [60], *Cure* [17], *Chameleon* [23], *Rock* [18] and many more [41, 39, 33, 61]. Those schemes start from every data point assigned to its own cluster and then merge repeatedly the pairs of clusters according to a minimum distance criterion. *Birch* constructs the feature tree of clustering (cf-tree), where one node stands for a sub-cluster. The tree grows dynamically when a new data point comes. *Cure*, which is suitable for large-scale clustering, takes random sampling technique to cluster sample separately. *Rock* is an improvement of *Cure* that stands for numerical data. *Chameleon*, divides the original data into smaller clusters based on the \( k \)-nn graph\(^1\), and then the small clusters are merged, based on agglomerative criterion. On the other hand, *divisive* (top-down) or partitioning schemes, start with all data points in one cluster and then perform repeated bisections until a certain criterion function is optimized [9, 4, 24]. Previous work on graph partitioning has been done in [51, 50, 5, 3]. Moreover, a well known divisive clustering algorithm is (Principal Direction Divisive Partitioning) PDDP [9], which is based on PCA and is claimed to be very effective in clustering document collections. Bisecting \( k \)-means [24], a simple variation of \( k \)-means, is another divisive clustering approach.

1.2 Motivation and Related Work

**Motivation** The research for this thesis has been motivated by the work done by C. D. Meyer and C. D. Weissel in [37] and their idea to develop a technique for

\(^1\)The \( k \)-nearest neighbor graph is a graph in which two vertices \( u \) and \( v \) are connected by an edge, if the distance between \( u \) and \( v \) is among the \( k \)-th smallest distances from \( u \) to other vertices
1.2. Motivation and Related Work

using the evolution of the system in order to find out its initial structure. This idea was in its turn based on the on the variable aggregation theory of H. Simon and A. Ando [53].

H. Simon and A. Ando provided a way of understanding the sort and long term behavior of an economic system with a *Nearly Completely Decomposable* (NCD) structure. This means that the variables of the system are organized in a hierarchical way into blocks, sub-blocks and so on, such that the interactions between variables of the same block are stronger that interactions between variables of different blocks. A major conclusion of Simon-Ando theory is that the smaller and more cohesive sub-systems tend toward a local equilibrium long before a global equilibrium. The observation that many complex systems in the nature, such as brain organization systems and biological systems, share the property of being NCD, turned Simon-Ando theory into a very useful framework that can be applied almost every domain of science.

In the majority of applications, the structure of the system is known and the point of interest are the various stages the system passes through on the way to reaching a state long-term equilibrium. However, in [37] the authors address the problem from the another direction. In particular, they propose a solution to the well known problem of consensus clustering, named *Stochastic Data Clustering*. They propose two alternative algorithms that work as follows: First, they store the accumulated results of various clustering algorithms, in a consensus similarity matrix $S$, where the value of $s_{ij}$ equals the number of times data elements $i$ and $j$ are clustered together. The fact the values of more relevant entries in the $S$ are larger (NCD structure), implies that Simon-Ando theory can be applied. Then, they convert the matrix $S$ into a doubly stochastic matrix. Specifically, consider the *doubly stochastic*, nearly completely decomposable matrix.

$$
P = \begin{bmatrix}
P_{11} & P_{12} & \cdots & P_{1k} \\
P_{21} & P_{22} & \cdots & P_{2k} \\
\vdots & \vdots & \ddots & \vdots \\
P_{k1} & P_{k2} & \cdots & P_{kk}
\end{bmatrix}
$$

where the elements of the diagonal blocks of the diagonal blocks $P_{ii}$ are much larger than the elements in the off-diagonal blocks. Let $x_0$ be a random probability row vector and consider the evolution equation $x_t = x_{t-1} P$. Simon-Ando theory states that as $t$ increases, $x_t$ passes through well-defined stages:

- Initially, the large values in the $P_{ii}$ blocks cause relatively large changes in $x_t$.
- Since $P$ is doubly stochastic, as $t \to \infty$, $x_t \to$ the uniform probability distribution vector.
• Between these two extremes, the elements of $x_t$ accumulate near $n$ distinct values, where $n$ is the number of eigenvalues of $P$ near one.

This last point is essential to using Simon-Ando theory as a data clustering technique, since it allows us to cluster the original data, based on the clustering of the corresponding probabilities in $x_t$. The basic requirement is that the matrix $S$ contains the data, should be converted into doubly stochastic.

The novelty of the Stochastic Data Clustering method [37], lies in the fact that it uses a doubly stochastic normalization, in order to keep track of the local convergence by using an early stopping random walk. Although, this idea gives a useful insight on how data should be clustered, it suffers from three serious disadvantages. First of all, in the beginning of the process, the computation of a large number of clustering results, adds significant workload to the algorithm. Secondly, the algorithm cannot be applied directly in traditional data clustering problems, where the data are modeled in the form of similarities, because it demands that the data matrix has a block diagonal form (the clusters are well separable). This is why it is proposed as a consensus clustering technique. Finally, it completely ignores the hierarchical structure of the data. The existence of any hierarchy could harm the effectiveness of the method, since it affects the block diagonal form of the data matrix.

In this work, we adopt the above mentioned approach together with its rich mathematical formalization, in order to overcome the limitations and move one step beyond what is achieved in [37]. Our goal is to detect hierarchical nested structures on any data that can be represented in the form of similarities. We are going to use the NCD property in order to find less informative partitions in the higher levels of the hierarchy and then step forward to more detailed lower partitions by dividing the whole clustering problem into smaller ones.

**Related Work**  The theory of NCD systems has been applied in a variety of computer science tasks. Courtois [11], was the first to introduce the theory of NCD systems on the field of computer science, by applying it in queuing systems. He also developed the formal mathematical theory. More recent work includes the research done by Nikolakopoulos et al. [47, 46, 48, 45, 44] on ranking and ranking-based recommendations. Unlike other information retrieval methods that ignore the hierarchical structure of data, those methods are build to exploit the concept of NCD and achieve remarkable results both in terms of quality and efficiency.

C. D. Meyer and C. D. Weissel, as we discussed mentioned, used the theory on the evolution of NCD systems to solve the problem of consensus clustering. In a following work [35], is proposed an iterative technique, that refines the data matrix in way that encourages its block-diagonal form. This technique is a flexible,
1.3. Our Contribution

exploratory method for determining the number of clusters. Its framework can be adapted to use any clustering algorithms or dimension reductions.

To the best of our knowledge, the most similar approach to [37] is Power Iteration Clustering (PIC) [32], a graph clustering method that aims at finding a very low-dimensional embedding of a dataset using truncated power iteration on a normalized pair-wise similarity matrix. This approach is more general and efficient from Stochastic Data Clustering, since it uses a single measure of similarity instead of many clustering results. The subsequent researches [31] and [20], focus on the high applicability of PIC in several domains.

Last but not least, related to our work can be considered the Markov Clustering Algorithm (MCL). It is a graph clustering algorithm that also applies random walks upon the graph, in order to discover where the flow tends to gather, and therefore, where clusters are [55].

1.3 Our Contribution

We present a simple and fully parallelizable divisive hierarchical clustering framework called Hierarchical Stochastic Clustering (HSC), that acts in two stages. In the first stage, it finds a primary hierarchy of clustering partitions in a dataset. In the second stage, feeds a clustering algorithm with each one of the clusters of the very detailed partition, in order to settle the final result. The output is a hierarchy of clusters. In other words, we offer a general scheme of clustering that works as “preconditioner”² for data clustering algorithms and improves the quality of their results. Figure 3.2 provides a schematic representation of the framework.

The main method, named (HSC) algorithm, operates random walks on a sparse graph in which nodes represent data items, and weighted edges represent similarities among the data items. The output of the algorithm is a primary hierarchy of clusters. We provide the experimental evaluation of the method. This includes tests on the inner parameters and comparison with well known clustering algorithms.

The characteristics of our work:

- The introduction and development of the HSC algorithm. An extensive analysis of its mathematical characteristics concerning both the modeling and the computation.

²In semi-numerical and numerical algorithms, preconditioning is the application of a transformation, called the preconditioner, that brings a given problem into a conditions that is better suited for some solution method.
• Unlike other clustering algorithms, it does not make any assumption about neither the number of hierarchical levels nor the number of clusters. The number of levels and the number of clusters in each level are determined by the algorithm. Practically, this property makes it more effective because in realistic clustering problems, this information is usually unknown.

• We optimize HSC by introducing a lighter alternative of Stochastic Complementation, that speeds up the algorithm significantly without harming the clustering quality. This is shown experimentally. We also propose some other optimizations.

• We prove that the top-down strategy can lead to better performance on the grounds that the gradual decomposition of the problem leads to more qualitative low level clusters and because the division into sub-problems reduces drastically the time complexity of the algorithm that acts in the lower level.

### 1.3.1 Organization

The rest of the thesis is organized as follows:

Chapter 2 describes the data modeling techniques that are used and presents the basic concepts and background material. It includes the description of the concepts of Double Stochasticity, Near Complete Decomposability and Stochastic Complementation.

In Chapter 3, the overall method is presented in detail, together with algorithms, examples and further optimizations. Moreover, we introduced the idea of Diagonal Complementation whose effect is to optimize the performance of the method.

Chapter 4 provides the experimental evaluation of the method. This includes tests on the inner parameters and comparison with well known clustering algorithms.

Finally, Chapter 5 contains the concluding remarks about the topics covered in the thesis and future research directions.
1.3.2 Notation

| Symbols        | Definitions                                                                 |
|----------------|-----------------------------------------------------------------------------|
| $\pi$, $\pi^T$| a vector and its transpose                                                  |
| $A$            | a similarity matrix                                                         |
| $S$            | a doubly stochastic matrix                                                 |
| $s_{ij}$       | the $ij$-th entry of matrix $S$                                             |
| $S_{ij}$       | the $ij$-th sub-block of matrix $S$                                         |
| $G = \{V,E\}$ | a graph or network, the set of its nodes and its edges                     |
| $e = (u,v)$    | the edge $e \in E$ from node $u$ to $v$                                     |
| $w(u,v)$       | the weight of the edge $e = (u,v)$                                         |
| $d_u$          | degree of node $u$                                                          |
| $[1,n]$        | a set of numbers $\{1,2,\ldots,n\}$                                       |
| $l$            | hierarchical clustering level                                               |
| $n_l$          | the number of clusters of the $l$-th hierarchical level                    |
| $C_1, \ldots, C_m$ | a hierarchy of $m$ levels, each set $C_l$ represents a partition          |
| $Q^l_1, \ldots, Q^l_{n_l}$ | a partition that belongs to the $l$-th level of the hierarchy,             |
|                | each set $Q^l_i$ represents a cluster and $\forall Q^l_i \in C_l$        |
| $D(r)$         | a diagonal matrix, where $r$ is the vector                                 |
| $S^*_i$        | the stochastic complement of the sub-block $S_{ii}$ of $S$                 |
| $S_i$          | the matrix obtained by deleting the $i$th row and $i$th column of blocks from $S$ |
| $S_{i*}$       | the $i$th row of blocks of $S$ with $S_{ii}$ removed                      |
| $S_{*i}$       | the $i$th column of blocks of $S$ with $S_{ii}$ removed                    |
| $\text{diag}(S_{11}, S_{22}, \ldots, S_{nn})$ | a block-diagonal matrix with $S_{11}, S_{22}, \ldots, S_{nn}$ diagonal blocks |
| $\text{Tr}(E)$ | is the trace of matrix $E$                                                 |
Chapter 2

Preliminaries

In this Chapter, we initially present the data modeling approach that we follow (Section 2.1). Then, we describe the method that we use in order to transform the matrix into doubly stochastic (Section 2.2). Finally, we define the concepts of Near Complete Decomposability and Stochastic Complementation and explain how our method depends on them (Section 2.3 and Section 2.4).

Given $k$ data points represented by the integers from 1 through $k$, our goal is to build a hierarchy of $m$ levels $C_1, \ldots, C_m$. Each level $l$, where $l = \{1, \ldots, m\}$, consists of $n_l$ disjoint clusters $Q_{l1}^1, \ldots, Q_{ln_l}^l$. To achieve this, we follow a top down approach, where we start with all data points belonging to one cluster in the first level ($l = 1$), and then we split it recursively as we move down the levels of the hierarchy ($l > 1$). Hierarchical clustering solutions, are usually represented by trees called dendrograms, in which closely related pairs of vertices have common ancestors that are lower in the dendrogram than those of more distantly related pairs.

2.1 Similarity Matrix

There are a lot of clustering algorithms that are based on similarities between the data points. In the case that the data points represent documents, for example, one could compute content-based similarity values for all pairs of documents and use the similarity matrix as a basis for the clustering, attempting to group together data points that are very similar to each other. The higher the similarity, the stronger the need to cluster the data points together. Computing such similarities is not necessarily simple, and in some cases evaluating them may turn out to be a task even more complex than the clustering once the similarities are known. The construction

\footnote{For simplicity, when we refer to the first level (or one level) we omit the index of the level and we use the notation $Q_i$ for the $i$th cluster and $n$ for the number of clusters of that level.}
Chapter 2. Preliminaries

Figure 2.1: The similarity matrix induced by cosine similarities on the left and after applying $k$-nn (with $k = 50$) on the right.

of the similarity matrix requires some primary steps of preprocessing to be done by the user, depending on the nature of the data [7]. The number of similarity measures used in the literature is very large and there is a diversity of studies that evaluate their performance in different kinds of clustering problems [19].

A common similarity measure for data with multiple features, is *cosine similarity*. It computes the $l_2$-normalized dot product of vectors. That is, if $x$ and $y$ are row
vectors, their cosine similarity is defined as:

\[
\frac{\mathbf{x} \mathbf{y}^T}{\|\mathbf{x}\| \|\mathbf{y}\|}
\]

The resulting similarity ranges from -1 meaning that the vectors point in the opposite direction, to 1 meaning the vectors point in the same direction, with 0 indicating orthogonality (de-correlation), and in-between values indicating intermediate similarity or dissimilarity. However, most of the times the problem with most traditional similarity measures is that their values tend to the middle of their range. This is well noted in [35], as well as in many other researches. In order to avoid this limitation and obtain a sparse graph representation, we use the concept of \( k \)-nearest neighbors graph (\( k \)-nng) [14]. The \( k \)-nng is a graph in which two vertices \( u \) and \( v \) are connected by an edge, if the distance between \( u \) and \( v \) is among the \( k \)-th smallest distances from \( u \) to other vertices. This kind of sparsification, transforms the similarity distributions so that they contain more values near the extremes. The Figures 2.1 and 2.2 depicts a similarity matrix and the histogram of similarity values before and after the transformation.

Modeling data items as a graph, is very common in many clustering algorithms. There are many examples of methods can be used to find a graph representation. Agglomerative hierarchical clustering algorithms based on single link, complete link, or group averaging method, operate on a complete graph. Other algorithms, use a similarity threshold and the concept of shared neighbors in order to sparsify the graph [7]. The advantage of graph-based methods is that it can reduce the
high-dimensionality of the feature space via a similarity metric. It can also reflect non-local properties of the data.

In the case of networks (simple or weighted), the data are represented by a connectivity matrix that contains 1 in the positions of adjacent vertices and 0 otherwise or the weights of the vertices in the weighted case.

To sum up, in our approach, the data are represented by pairwise non negative similarities, stored in a matrix similarity matrix $A$. The element $a_{ij}$ of $A$ denotes the similarity score between data points $i$ and $j$. Notice that a similarity graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ can give an alternative representation of the similarity matrix, with each node $v \in \mathcal{V}$ represent a data point and each weighted edge $(u, v) \in \mathcal{E}$ a similarity between nodes $u$ and $v$. The problem of hierarchical clustering can now be reformulated using $\mathcal{G}$: we want to find partitions of the graph such that the edges between different groups have very low weights and the edges within a group have high weights. The partitions that belong in higher levels of the hierarchy are more detailed that those in the lower levels. In the Figure 2.3 there is a simple example of a similarity graph that describes a friendship network. The data are modeled such that the corresponding similarity matrix coincides with the connectivity matrix of the network.

![Figure 2.3: Application of HSC algorithm in a friendship network. 2.3α′ and 2.3β′ indicate respectively the first and the second level partition found by the algorithm. The graph has been laid out using the Force Atlas algorithm, of the open source software Gephi [6].](image)

The similarity matrix $A$ is by construction symmetric with strictly non zero diagonal elements. We will assume from now on that the similarity graph is strongly connected. When graph is divided into independent clustering problems, we treat each
of them separately. For example, if the similarity graph consists of more than 
one connected components then each of them constitutes a different cluster and a 
clustering algorithm can be applied independently on each of them in order to find 
further partitions. The strong connectivity of the similarity graph guarantees that 
the similarity matrix $A$ is irreducible.

## 2.2 Doubly Stochastic Normalization

If a graph has the appropriate structure, a random walk can be generated on it by 
applying a suitable scaling to the similarity matrix and transform it into a stochastic 
matrix\(^2\). This transformation is obtained by a scaling induced by a diagonal matrix, 
$D$, of column sums so that $P = AD^{-1}$ is column-stochastic. According to [37], an 
alternative method of generating a random walk on $G$ is to apply a diagonal scaling 
to both sides of $G$ to form a doubly stochastic matrix $S = DAE$.

The Sinhorn-Knopp (Sk) algorithm\(^2\) is the simplest method for finding a doubly 
stochastic scaling of a nonnegative matrix, $A$. It does this by generating a sequence 
of matrices whose rows and columns are normalized alternately. The algorithm can 
be thought of in terms of matrices

$$A_0, A_1, A_2, \ldots$$

whose limit is the doubly stochastic matrix, or in terms of pairs of diagonal matrices

$$(D_0, E_0), (D_1, E_1), (D_2, E_2), \ldots$$

whose limit gives the desired scaling of $A$. Suppose that $S = D(r)AD(c)$ is doubly 
stochastic. Manipulation of the identities $Se = e$ and $S^T e = e$ gives

$$c = D(A^T r)^{-1}e, r = D(Ac)^{-1}e$$

which suggests the fixed point iteration

$$c_{k+1} = D(A^T r_k)^{-1}e, r_{k+1} = D(Ac_{k+1})^{-1}e$$

If $A$ is symmetric, as it is in our case, then it is natural to look for a diagonal 
matrix $D$ such that $DAD$ is doubly stochastic [25]. We can do this by using the Sk

\(^2\)Each column of a column-stochastic matrix sums to 1
algorithm. If \( D(r)AD(c) \) is doubly stochastic then so is its transpose \( D(c)AD(r) \).

During the iteration, though, symmetry is lost, so, an alternative approach is to generate a sequence of symmetric iterates. The symmetric analogues of 2.2 and 2.2 are

\[
x = D(Ax)^{-1}e
\]

and

\[
x_k = D(Ax_{k-1})^{-1}e
\]

The problem of symmetric balancing is also considered in [26], and it is solved by using a Gauss-Seidel-Newton method.

The similarity matrix is normalized into doubly stochastic as in [37], by performing the following scaling

\[
S = DAD,
\]

where \( D \) is diagonal with positive diagonal elements [37, 25].

**Definition 1.** (see [54] and [37]) A nonnegative \( n \times n \) is said to have total support if \( S \neq 0 \) and if every positive element of \( S \) lies on a positive diagonal, where a diagonal is defined as a sequence of elements \( s_{1\sigma(1)}, s_{2\sigma(2)}, \ldots, s_{n\sigma(n)} \) where \( \sigma \) is a permutation of \( \{1, 2, \ldots, n\} \).

**Theorem 1.** (Sinkhorn-Knopp) If \( A \in \mathbb{R}^{n \times n} \) is nonnegative then a necessary and sufficient condition that there exists a doubly stochastic matrix \( S \) of the form \( DAE \) where \( D \) and \( E \) are diagonal matrices with positive main diagonals is that \( A \) has total support. If \( S \) exists then it is unique. \( D \) and \( E \) are also unique up to a scalar multiple if and only if \( A \) is fully indecomposable.

**Lemma 1.** (see Csima and Datta [12]) Let \( A \) a fully indecomposable symmetric matrix. Then, there exists a diagonal matrix \( D \) such that \( DAD \) is doubly stochastic.

**Theorem 2.** (Minc [38, p. 82]) An \( n \times n \) matrix \( A \) is partly indecomposable if there exist permutation matrices \( B \) and \( C \) such that

\[
BAC = S = \begin{bmatrix} X & Z \\ 0 & Y \end{bmatrix}
\]

where \( X \) and \( Y \) are square. If no such \( B \) and \( C \) exist, then \( S \) is fully indecomposable.

**Definition 2.** (Minc [38, p. 82]) Two matrices \( X \) and \( Y \) are permutation equivalent, or \( p \)-equivalent, if there exist permutation matrices \( Q \) and \( \hat{Q} \) such that \( X = QY\hat{Q} \)

**Definition 3.** (Minc [38, p. 86]) A nonnegative matrix is fully indecomposable if and only if it is \( p \)-equivalent to an irreducible matrix with positive main diagonal.

The similarity matrix of our model, \( A \), is by construction irreducible with positive main diagonal and is \( p \)-equivalent to itself since it holds that \( A = IAI \). As a result,
A is fully indecomposable (see Definition 3). Also, it is by construction symmetric. So, it can be converted into doubly stochastic (see Lemma 1).

It is important to mention that the doubly stochastic normalization does not harm either the zero structure or the symmetry of the data, as it is proven in [37]. The matrix $S$ will have the same zero structure with $A$ because since $s_{ij} = d_{ii}d_{jj}a_{ij}$, and both $d_{ii}$ and $d_{jj}$ are positive, $s_{ij} = 0$ when $s_{ij} = 0$. This means that $S$ is also irreducible with non zero diagonal elements. Moreover, $S$ will be symmetric because both $D$ and $A$ are symmetric (see Equation 2.5).

The matrix $S$ provides an alternative method of generating a random walk on $G$. We will refer to it as *doubly stochastic transition matrix*. The derived Markov chain is irreducible, because $S$ is irreducible, with non periodic states, because $S$ has non zero probabilities in the main diagonal. These two properties ensure that the chain is ergodic (or that the matrix $S$ is primitive) and thus, it has a unique stationary distribution. Moreover, as we know from the theory of Markov chains, for a doubly stochastic transition matrix the stationary distribution is the uniform distribution. More precisely, it holds that

$$\pi^\top = \pi^\top S$$

where $\pi^\top = \left[ \frac{1}{k} \ \frac{1}{k} \ \ldots \ \frac{1}{k} \right]^\top$. Notice that the graph $G$ can be slightly modified by replacing the weights with the normalized weights arisen from the doubly stochastic normalization. After this modification we can alternatively define the above mentioned Markov chain as the random walk on the modified graph $G$.

### 2.3 Near Complete Decomposability

According to H. Simon [53] all viable systems, physical, social, biological, artificial, share the property of having a near decomposable architecture: they are organized into hierarchical layers of blocks, sub-blocks and so on, in such a way that interactions among elements belonging to the same block are much more than interactions among elements belonging to different blocks. According to that theory, if a Markov chain is NCD if there is a partition of classes $C = \{\mathcal{Q}_1, \mathcal{Q}_2, \ldots, \mathcal{Q}_n\}$ which classifies its state space in such way that $\mathcal{Q}_i$’s are very weakly connected.

---

3For simplicity, we use the same notation for the clustering of data points and the partition of states of the Markov chain, $C_j, Q_j, n_j$, etc. because they represent the same thing.
If we arrange the rows and columns of the transition matrix $S$ according to the partition $C$, the off-diagonal blocks $S_{ij}$ in the transition matrix

$$
S = \begin{bmatrix}
S_{11} & S_{12} & \ldots & S_{1k} \\
S_{21} & S_{22} & \ldots & S_{2k} \\
\vdots & \vdots & \ddots & \vdots \\
S_{k1} & S_{k2} & \ldots & S_{kk}
\end{bmatrix}
$$

of a finite aperiodic chain have sufficiently small magnitudes, then the closely coupled subclasses associated with diagonal blocks $P_{ii}$ must tend toward a local equilibrium long before a global equilibrium.

Generally speaking, in clustering scenarios the similarity values between data points that belong to the same cluster are larger than those between data items that belong to different clusters. When the clusters are hierarchically organized, the matrix $S$ can be partitioned in multiple ways, according to how strict one is with the within cluster similarities (see for example Figure 2.3). Motivated by this observation, we go beyond a single partition and we make use of the NCD property in order to look for a hierarchy or sequence of partitions, $C_1, C_2, \ldots, C_m$, where $Q_1^l, Q_2^l, \ldots, Q_m^l$ are the classes of $C_j$. One way to do this, is to consider every sub-block of $S_{ii}$ of $S$ as an independent Markov chain that is described by a stochastic matrix $S_{ii}^\star$. If the NCD property exists in the smaller chains, their state spaces can be partitioned further so that the partition $C_j$ contains the sub classes of $C_{j-1}$ and so on. What remains to explain is the exact way the sub stochastic $S_{ii}$ diagonal block matrices will be converted into the stochastic $S_{ii}^\star$ and how double stochasticity is maintained. This is explained in detail in Section 2.4.

Let us define the stochastic process

$$
\pi_i^T = \pi_{i-1}^T S
$$

The Simon-Ando theorems [53] predict that $S$ is NCD, as $t$ increases $\pi_i^T$ passes through well defined stages.

- **Short-run and middle run**: The large values in the $S_{ii}$ blocks cause relatively large changes in $\pi_i^T$. This means that even for small values of $t$ structure of $\pi_i^T$ reflects the stationary probability vectors of the stochastic complements $S_{ii}^\star$ of the blocks $S_{ii}$, namely the vectors $\sigma_i^T$ (see Equation 2.11). In other words, the elements of $\pi_i^T$ accumulate near $k$ distinct values, where $k$ is the number of eigenvalues of $S$ near one. The only difference between short-run and middle run is whether the elements of $\pi_i^T$ stay at approximately the same value for a number of iterations or move together towards the uniform probability distribution (see [37] for more details).
• Convergence: Since $S$ is doubly stochastic, as $t \to \infty$, $\pi_\top t$ approaches the uniform distribution.

When $S$ is hierarchically structured, the blocks that are lower in the hierarchy approach first the uniform distribution, and with the passage of time, they hand over the baton to their super-blocks, i.e. the blocks that they belong to. This is justified by the fact that the probability that is spread outside the block in the hierarchical case, is not spread uniformly to the other blocks. The blocks that have common ancestor with the current block are more likely to be reached. Notice that the fact that the blocks lower in the hierarchy are more mixed that their super blocks leads us to the conclusion that the short-run and middle-run stages are not well defined and last less time than those of their super blocks.

2.4 Stochastic Complementation

Stochastic Complementation is a technique for reducing an irreducible Markov chain with a large number of states to a smaller chain without losing important characteristics. The definition and the probabilistic interpretation of stochastic complementation were introduced in [36].

Each diagonal block $S_{ii}$ of $S$ has a stochastic complement defined by

$$S_{ii}^* = S_{ii} + S_{i*}(I - S_i)^{-1}S_{i*}$$

(2.10)

where $S_i$ is the matrix obtained by deleting the $i$th row and $i$th column of blocks from $S$, $S_{ii}$ is the $i$th row of blocks of $S$ with $S_{ii}$ removed, and $S_{i*}$ is the $i$th column of blocks of $S$ with $S_{ii}$ removed. The final block diagonal matrix will is constructed as follows, $S^* = \text{diag}(S_{11}^*, S_{22}^*, \ldots, S_{nn}^*)$.

In [37] proven that, if $S$ is an irreducible doubly stochastic matrix, then each stochastic complement $S_{ii}^*$ is also an irreducible doubly stochastic matrix. Therefore, each stochastic complement has a uniform stationary distribution vector

$$\sigma_i^\top = \begin{bmatrix} \frac{1}{r_i} & \frac{1}{r_i} & \cdots & \frac{1}{r_i} \end{bmatrix}$$

(2.11)

where $r_i$ indicates the number elements in $\sigma_i^\top$.

Since $S$ is doubly stochastic, it holds that all the eigenvalues in its spectrum are real and reside in the interval $[-1,1]$. Moreover, the primitivity of $S$ (irreducible with at least one non zero diagonal element), guarantees that the largest eigenvalue, $\lambda_1$, is equal to 1 and its simple. The NCD property is captured in the spectrum of $S$. 
in a way that there exist $n$ eigenvalues very close to 1, i.e. there are $n$ eigenvalues $\lambda_1, \lambda_2 \ldots \lambda_n$ in the Perron cluster [13]. In fact, the bigger the gap between the eigenvalues of the Perron cluster and the rest of the eigenvalues is, the more well defined the $n$ clusters are.

**Definition 4.** Let $S$ be an $n \times n$ symmetric, stochastic matrix with eigenvalues, including multiplicities, of $1 = \lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \ldots \geq \lambda_n$. If the largest difference between consecutive eigenvalues occurs between $\lambda_k$ and $\lambda_{k+1}$, the set of eigenvalues $[1, \ldots, \lambda_k]$ is called the Perron cluster of $S$. If two or more pairs of eigenvalues each have differences equal to the largest gap, use the smallest value $k$ to choose $\lambda_k$. The larger the gap, the more well defined the cluster.

In hierarchically structured data, it is not expected that the clusters will be well defined, because the existence of the hierarchy acts as a mixing factor among them. Intuitively, there will be further gaps that divide the Perron cluster and indicate less concise partitions of the data. Considering the hierarchy of $m$ levels, there will be $m - 1$ gaps in the Perron cluster which define $m - 1$ clusters of eigenvalues. The number of eigenvalues in each of them will be $n_1, n_2 \ldots n_m$ in descending order, correspond the number of the clusters in each level. In the example of Figure 2.4, we plot the eigenvalues of a 3-level hierarchical graph. Except for the largest gap that defines the Perron cluster, there are two more gaps inside the Perron cluster indicating that there exist two more upper levels. Subsequently, the Perron cluster of $S$ and the way that it is structured, most of the times, gives a powerful insight about how the data is actually structured. This hidden property plays a key role in the dynamical behavior of the system described by $S$ (see Section 2.3 for more details).

In this Chapter we described how the data of the problem are modeled and defined their mathematical properties. Notice that these properties, i.e. the exact NCD structure, the structure of the Perron cluster and so on, are not known beforehand. This is latent information that essentially drives our method. What we plan to do next is to observe the evolution of the distribution vector in order to recognize the clusters of proximate states. Then, we are going to reduce the system into sub systems in order to reach deeper levels in the hierarchy.
2.4. Stochastic Complementation

\textbf{Figure 2.4:} $\alpha'$ is a graph with three hierarchical levels. The first level consists of 2 clusters, the second level of 6 clusters and the third level of 9 clusters. $\beta'$ is a plot of the 50 (greatest in magnitude) eigenvalues of the graph. The structure of the Perron cluster reflects the structure of the graph. The graph was constructed by using LFR benchmarks and was laid out by using the Force Atlas algorithm, of the open source software Gephi [6]
Chapter 3

Hierarchical Stochastic Clustering

In this Chapter, we present our framework, named Hierarchical Stochastic Clustering (HSC) (Section 3.1). Then, we introduce an alternative method of Stochastic Complementation, named Diagonal Complementation and we propose some further optimizations (Section 3.3).

3.1 Algorithm

The Algorithm FindCluster (1), as in [37], begins using a seeding vector $\pi_0^\top$ with zeros in all states except for one, the seeding state. It tracks the evolution of $\pi_t^\top$ before it converges to the stationary distribution, in a moment $t$ in which the states that belong to the class of the seeding state approach the short-run and middle-run stages. The elements in $\pi_t^\top$ that remain for a long time closest to the seeding data point belong to the cluster. The process of identifying a single cluster is formulated in Algorithm 1.

Parameter $\text{repcl}$ plays an important role in the determination of a cluster. The final cluster is determined when it remains the same for $\text{repcl}$ number of iterations. Intuitively, this means that the changes in $\pi^\top$ are very small or insignificant for $\text{repcl}$ number of steps, a situation that characterizes the short-run and middle-run stages. The goal is to discover well-defined clusters in multiple levels. When clusters are well-defined, the short-run and middle-run stages last a long time and we can capture them more easily by setting the parameter $\text{repcl}$ to be sufficiently large. This conclusion is justified by the theory about the dynamical behavior of a system. When the clusters of the first level are determined, we focus on each one of them independently and we apply in the corresponding sub-block stochastic complementation in order to partition them in the same way.

Figure 3.1 shows $\pi_t^\top$ when each of the cluster in the hierarchy is determined. The
Algorithm 1 FindCluster

Input: $S$, $\text{maxit}$, $\text{repcl}$, $\text{mincl}$, $\text{seed}$, $\alpha$

Output: $Q$

1. $\pi_0^T \leftarrow [0 \ldots 0]^T$, $\pi_0^T[\text{seed}] \leftarrow 1$
2. $Q \leftarrow \emptyset$, $Q_{\text{prev}} \leftarrow \emptyset$, $\text{count} \leftarrow 0$
3. repeat
4. if ($t = \text{maxit}$) then return $\emptyset$
5. end if
6. $\pi_{t+1}^T \leftarrow a \pi_t^T S + (1 - a) \frac{1}{n} e^T$
7. Sort $\pi_{t+1}^T$ in ascending order. Find the maximum gap and create a cluster $C$ with the elements after the gap.
8. if ($Q \equiv Q_{\text{prev}}$) then $\text{count} \leftarrow \text{count} + 1$
9. else $\text{count} \leftarrow 0$
10. end if
11. $t \leftarrow t + 1$, $Q_{\text{prev}} \leftarrow Q$
12. until $\text{count} = \text{repcl}$
13. if ($\text{seed} \in Q$) and ($|Q| \leq \text{mincl}$) then return $Q$
14. else return $\emptyset$
15. end if

Algorithm 2 HSC

Input: $S$, $\text{maxit}$, $\text{repcl}$, $\text{mincl}$, $\alpha$

Output: $C_1, \ldots, C_m$

1. $i \leftarrow 1$
2. $Q_i \leftarrow \{1, \ldots, n_1\}$
3. $C_i \leftarrow Q_i$
4. while $C_i \neq \emptyset$ do
5. for every cluster $Q_i^j$ in $C_i$ do
6. $S \leftarrow Q_i^j$
7. repeat
8. Choose a seed and remove it from the set $S$
9. Find the stochastic complement $S_{ji}^j$ of $Q_i^j$
10. $Q \leftarrow \text{FindCluster}(S_{ji}^j, \text{maxit}, \text{repcl}, \text{mincl}, \text{seed}, \alpha)$
11. Add $Q$ in the set $C_{i+1}$
12. Remove the elements in $Q$ form the $S$
13. until $S \equiv \emptyset$
14. end for
15. $i \leftarrow i + 1$
16. end while
3.1. Algorithm

Figure 3.1: **The evolution of** $\pi_t^T$. Shows $\pi_t^T$ when each of the cluster in the hierarchy is determined. The dataset that we used is the dataset of the Figure 2.3. 3.1α': first level, 3.1β': second level

dataset that we used is the dataset of the Figure 2.3. The first level (3.1α', 2.3α') consists of two clusters. In the second level one of the clusters, the red cluster of the first level is split (3.1β', 2.3β'), as a result, it consists of three clusters.

We are looking for a hierarchy of different partitions $C_1, C_2, \ldots, C_m$ by adopting a top-down approach; we start with one cluster and we split it recursively. We obtain the level $C_j$ by finding the sub clusters of every cluster $Q_{i-1}$ in the level $C_{j-1}$. In order to achieve this, we need its stochastic complement $S_H$. The pseudo-code is formulated in the Algorithm 2.

Our method has the advantage of not including meaningless clusters in the hierarchy. The Algorithm 1, does not return a cluster in the cases that the size of the cluster is less than $\mincl$ and the number of iterations becomes greater than $\maxit$ as in [37]. Those two parameters are used in order to avoid deceptive clusters.
Therefore, if the seeding set $S$ runs out of seeds before finding any sub clusters, it means that the cluster $\mathcal{C}_j$ cannot be divided further. The procedure will stop in a level that contains no clusters.

### 3.1.1 Regularization

The newly introduced parameter $\alpha$, acts as a regularization in the random walk and it plays a role similar to the damping parameter of PageRank [29]. The final Markov chain, is obtained by perturbing the doubly stochastic transition matrix induced by the similarities between data points, $S'$, with a regularization factor $\frac{1}{k}ee^T$ that spreads uniformly a proportion $1-\alpha$ of the probability, as follows ¹

$$S = \alpha S' + (1-\alpha)\frac{1}{k}ee^T,$$  

where $k$ is the number of data points, and the final Markov process is defined as follows

$$\pi^T_{t+1} \leftarrow \alpha \pi^T_t S' + (1-\alpha)\frac{1}{k}e^T.$$  

When $\alpha$ approaches 1 the Markov process is closer to the original one - the process that arises directly from the data similarities - and this suggests that $\alpha$ should be chosen as 1, or as close to 1 as possible. Moreover, as we know from [8] the number of iterations required for the power method to converge grows with $\alpha$. Unlikely to PageRank, this fact is sometimes convenient for our method, since the slow convergence facilitates the identification of short-run and middle-run stages.

The final $S$ is irreducible as a convex combination of two irreducible matrices and has apparently at least on non diagonal element. The primitivity of $S$ guarantees the convergence of the power method. As stated before, the primitivity of $S'$ guarantees anyway the convergence and the absence of regularization does not harm the power method computationally. However, in the next section we propose an optimization in which the non zero value of $\alpha$ is necessary.

### 3.2 Framework

Our method can be used as a framework consisting of two stages. In the first stage, it finds a primary hierarchy of clustering partitions in a dataset. In the second stage, it feeds a clustering algorithm with each one of the clusters of the very detailed partition, in order to settle the final result. The output is a hierarchy of clusters.

¹We denote temporarily the doubly stochastic induced by the similarities as $S'$ in order to use the symbol $S$ for the final transition matrix.
3.3. Diagonal Complementation

As we stated previously, our method is not intended to be compared directly with hierarchical clustering algorithms but to provide a framework for clustering algorithms. Algorithm 2 belongs in the first stage and finds a primary hierarchy of clusters. Then, each of the clusters that belong to the last level of the hierarchy is fed to a clustering algorithm that acts in the lower level. Figure 3.2 provides a schematic representation of the overall framework.

We choose to create this framework for a simple reason. In the lower levels of the hierarchy the NCD property of the doubly stochastic diagonal blocks $S_{i1}, \ldots, S_{nn}$ tend to vanish. This means that either the data cannot be partitioned further, or the method cannot find further partitions because the short-run and middle-run stages are ambiguous. In the first case there is nothing to worry about, but in the second case Algorithm 2 can be considered ineffective, since in some cases other algorithms can find further partitions.

In the experimental evaluation we use several well known algorithms that take as input data similarities such as Spectal Clustering [43], Agglomerative clustering [39, 41], Birch [60] and $k$-means. The experimental results in the following chapter prove the effectiveness of the framework.

3.3 Diagonal Complementation

Stochastic complementation is computationally expensive since it includes an inversion. We propose a novel, lighter variant which we will refer to as Diagonal Complementation. We define the diagonal complement of $S_{ii}$ as

$$S_{ii}^* = S_{ii} + \text{diag}(S_{ii} e),$$

(3.3)

where $e$ is a column of ones and its size is whatever is appropriate for the context. Since the matrix $S$ is NCD, the factor $S_{ii} e$ is a vector with very small values. These values are added to the main diagonal of $S_{ii}$, and contribute to the self loops of the random walk by adding a very small probability. This modification, though, does not ensure that the $S_{ii}^*$ is irreducible. The regularization parameter of the equation 3.1 fixes the problem, so the equation 3.3 takes the form

$$S_{ii}^* = \alpha(S_{ii} + \text{diag}(S_{ii} e)) + (1 - \alpha)\frac{1}{k}ee^T$$

(3.4)

As a result, in the case of diagonal complementation the regularization parameter is necessary to be nonzero.

It is obvious that after diagonal complementation with regularization, every diagonal complement $S_{ii}^*$ is an irreducible matrix, as every node is directly connected.
Chapter 3. Hierarchical Stochastic Clustering

Figure 3.2: Framework schema
to every other node through $\frac{1}{k}ee^\top$. Furthermore, it is non periodic because of the non-zero diagonal. Therefore, $S_{ii}^*$ is primitive with a uniform stationary distribution vector. It remains to show that the diagonal complementation does not harm the double stochasticity of the diagonal complements.

**Theorem 3.** If $S$ is a doubly stochastic matrix then each diagonal complement $S_{ii}^*$ is a doubly stochastic matrix.

**Proof.** Let $e$ represent a column of all ones. First of all, we prove that the rows of a diagonal complement sum to one. Since the rows of $S$ sum to one the matrix $S_{ii} + \text{diag}(S_{*,i})$ is a row stochastic matrix the equation 3.5 holds

$$S_{ii}e = e$$
$$\alpha(S_{ii} + \text{diag}(S_{*,i}))e + (1 - \alpha)(\frac{1}{k}ee^\top)e = e$$

(3.5)

Next, we have to prove that the columns of a diagonal complement sum to one. This can be done by showing that $e^\top S_{ii}^* = e^\top$ in a similar way.

The experimental results in the next chapter show that diagonal complementation is more efficient and more effective that stochastic complementation.

**Further Optimization**

It is useful to notice that, in the case of many hierarchical levels, the complementation - both stochastic and diagonal - is a procedure that can be applied gradually. The computation of the complement of a block can be done by operating only to its super-block. It is not necessary to use the original matrix. In this way, we reduce even more the workload of the complementation phase in the lower levels.
Example

Doubly Stochastic Normalization

\[ A = \begin{pmatrix} 1 & 1 & 1 & 1 & \cdots & .139 \\ .221 & .327 & .273 & .179 \\ .135 & .048 & .139 & .189 & .140 & .161 \end{pmatrix} \rightarrow \]

\[ S = \begin{pmatrix} 1 \cdot 1 \cdot 1 \cdot 1 \cdot 1 \\ 1 \cdot 1 \cdot 1 \cdot 1 \cdot 1 \\ 1 \cdot 1 \cdot 1 \cdot 1 \cdot 1 \\ 1 \cdot 1 \cdot 1 \cdot 1 \cdot 1 \\ 1 \cdot 1 \cdot 1 \cdot 1 \cdot 1 \\ 1 \cdot 1 \cdot 1 \cdot 1 \cdot 1 \\ 1 \cdot 1 \cdot 1 \cdot 1 \cdot 1 \end{pmatrix} \]

Stochastic Complementation

\[ S_{sc} = \begin{pmatrix} .166 & .158 & .202 & .175 & .118 & .181 \\ .158 & .150 & .192 & .167 & .112 & .221 \\ .175 & .167 & .214 & .185 & .125 & .135 \\ .118 & .112 & .144 & .125 & .135 & .135 \\ .181 & .198 & .269 & .212 & .139 & .084 \\ .221 & .327 & .273 & .179 & .175 & .138 \\ .135 & .139 & .179 & .189 & .149 & .098 \end{pmatrix} \]

Diagonal Complementation

\[ S_{dc} = \begin{pmatrix} .166 & .158 & .202 & .175 & .118 & .181 \\ .158 & .150 & .192 & .167 & .112 & .221 \\ .175 & .167 & .214 & .185 & .125 & .135 \\ .118 & .112 & .144 & .125 & .135 & .135 \\ .181 & .198 & .269 & .212 & .139 & .084 \\ .221 & .327 & .273 & .179 & .175 & .138 \\ .135 & .139 & .179 & .189 & .149 & .098 \end{pmatrix} \]
Chapter 4

Evaluation

This Chapter provides the experimental evaluation of the method. This includes tests on the inner parameters and comparison with well-known clustering algorithms.

Algorithms In our comparisons we used the following algorithms:

\( \kappa \)-means: The number \( k \) of clusters to be generated is provided as input. Each cluster is represented by a center point, such as a centroid. The data items are partitioned among the \( k \) clusters, with each item assigned to the cluster with the closest centroid. Once this is done, centroids are recomputed for each cluster and the whole process is repeated until no centroids change.

Agglomerative clustering: Merges recursively the pair of clusters that minimally increase a given linkage distance. A linkage criterion is used to determine which distance to use between sets of observation. The \textit{Ward} criterion minimizes the variance of the clusters being merged. The average linkage (AL) criterion uses the average of the distances of each observation of the two sets.

Spectral clustering (SC): Applies \( \kappa \)-means clustering to a projection to the normalized Laplacian.

\textit{Birch}: Constructs a tree data structure with the cluster centroids in the leafs. These can be either the final cluster centroids or can be provided as input to another clustering algorithm such as agglomerative clustering.

Metrics We consider the stand-alone quality metrics of \textit{modularity}, \textit{conductance}, and \textit{coverage} \cite{2,42}, and we consider the information recovery metrics of \textit{Adjusted Rand score} (ARI) and \textit{Normalized Mutual Information} (NMI).
Let \( G = (V, E) \) be the undirected graph representing the similarity matrix \( S \). One of the most popular validation metrics for topological clustering, modularity, states that a good cluster should have a more than expected internal edges and a less than expected inter-cluster edges when compared to a random graph with similar characteristics. The modularity score for a clustering is given by

\[
\text{modularity} = \text{Tr}(E) - \|E^2\|, \tag{4.1}
\]

where \( E \) is a symmetric matrix whose element \( e_{ij} \) is the fraction of all edges in the network that link vertices in clusters \( i \) and \( j \), and \( \text{Tr}(E) \) is the trace of matrix \( E \), i.e., the sum of elements of its main diagonal. The modularity values can be either positive or negative and it is believed that the higher modularity values indicate stronger community structure. Although modularity has been shown to have a resolution limit \([16]\), some of the most popular clustering algorithms use it as an objective function.

The conductance of a cut compares the size of the cut and the number of edges in either of the two induced subgraphs. For a clustering \( C = \{Q_1, Q_2, \ldots, Q_k\} \) of a graph, the intra-cluster conductance is the minimum conductance value over all induced subgraphs is defined as follows

\[
\text{conductance}(C) = \min(\phi(Q_i)), \forall Q_i \in C, \tag{4.2}
\]

where

\[
\phi(Q) = \frac{\sum_{i \in Q} \sum_{v \not\in Q} w(u,v)}{\min(a(Q), a(Q'))} \tag{4.3}
\]

where \( w(u,v) \) is the weight of the edge \( \{u,v\} \), \( a(Q) \) is the sum of the weights of all edges with at least one endpoint in \( Q \) and \( C' = \{C - Q\} \).

The coverage of a partition \( C \) is given as the fraction of the weight of all intra cluster edges with respect to the total weight of all edges in the whole graph \( G \), as shown in the following equation

\[
\text{coverage}(C) = \frac{w(C)}{w(G)}, \tag{4.4}
\]

where \( w(C) = \sum_{i=1}^{k} w(u,v); u,v \in Q_i \) and \( w(G) \) is the total weight of all edges in the whole graph. Coverage values usually range from 0 to 1. Higher values of coverage mean that there are more edges inside the clusters than edges linking different clusters, which translates to a better clustering.

In order to compare the built-in hierarchical structure with the one delivered by our algorithm at each level, we adopt the NMI and ARI, two measures that has proven
to be reliable, since they are widely used as performance measures of network clustering algorithms [57, 21].

The NMI \( I_{\text{norm}}(X : Y) \) is defined as:

\[
I_{\text{norm}}(X : Y) = \frac{H(X) + H(Y) - H(X,Y)}{(H(X) - H(Y))/2},
\]

where \( H(X)(H(Y)) \) is the entropy of the random variable \( X(Y) \) associated with the partition \( \mathcal{C} \), whereas \( H(X,Y) \) is the joint entropy. This variable is in the range \([0,1]\) and equals 1 only when the two partitions and are exactly coincident [28].

The ARI is the corrected-for-chance version of the Rand Index. Given a set of \( n \) elements \( \mathcal{S} = \{o_1, \ldots, o_n\} \) and two partitions of \( \mathcal{S} \) to compare, \( \mathcal{X} = \{x_1, \ldots, x_r\} \), a partition of \( \mathcal{S} \) into \( r \) subsets, and \( \mathcal{Y} = \{y_1, \ldots, y_s\} \) a partition of \( \mathcal{S} \) into \( s \) subsets, define the following:

- \( a \), the number of pairs of elements in \( \mathcal{S} \) that are in the same subset in \( \mathcal{X} \) and in the same subset in \( \mathcal{Y} \).
- \( b \), the number of pairs of elements in \( \mathcal{S} \) that are in different subsets in \( \mathcal{X} \) and in different subsets in \( \mathcal{Y} \).
- \( c \), the number of pairs of elements in \( \mathcal{S} \) that are in the same subset in \( \mathcal{X} \) and in different subsets in \( \mathcal{Y} \).
- \( d \), the number of pairs of elements in \( \mathcal{S} \) that are different subsets in in \( \mathcal{X} \) and in the same subset in \( \mathcal{Y} \).

The Rand Index \( R \) is

\[
R = \frac{a + b}{a + b + c + d} = \frac{a + b}{\binom{n}{2}}
\]

The Adjusted Rand Index is

\[
\text{ARI} = \frac{\binom{n}{2}(a+b) - [(a+b)(a+c) + (c+d)(b+d)]}{\binom{n}{2}^2}
\]

Rand Index represents the frequency of occurrence of agreements over the total pairs, or the probability that \( \mathcal{X} \) and \( \mathcal{Y} \) will agree on a randomly chosen pair. ARI though, performs better than Rand Index in measuring agreement between two partitions in clustering analysis with different numbers of clusters. The value of ARI ranges between \(-1\) and \(1\).
Datasets  We adopted the realistic LFR benchmark graphs proposed in [27]. The benchmark graphs are binary with built-in hierarchical community structure and are widely used in many community detection studies.

| N  | k   | min k | max k | min c | max c | min C | max C | \( \tau_1 \) | \( \tau_2 \) |
|----|-----|-------|-------|-------|-------|-------|-------|-------|-------|
| 500| 20  | 50    | 50    | 80    | 100   | 200   | 2     | 1     |

Table 4.1: Fixed parameters for generating LFR graphs.

The graphs are of size \( N \), average degree \( k \) and maximum degree \( k_{\text{max}} \). There are two levels of clusters. The mixing parameters that we used \( \mu_1 \) and \( \mu_2 \), represent the fraction of links between the clusters of the corresponding level. The mixing parameters are varying according to the experiment. Generally, the higher values of the mixing parameters, the more difficult it is to extract the clusters of the level. The rest of the parameters of the generator are the following: node degrees and community sizes are governed by power law distributions with exponents \( \tau_1 \) and \( \tau_2 \) respectively, and cluster sizes vary in both small range \( (\text{min}c, \text{max}c) \) and large range \( (\text{min}C, \text{max}C) \). For some of the parameters we used the fixed values of the Table 4.1.

Finally, the real datasets that we used are the Glass and Ecoli (see [30] for more information).

The experimental evaluation was made on a computer with Intel Core i5-2450M 2.50GHz processor, 8 GB memory and operating system Ubuntu 16.04.

4.1 Model Parameter Tests

4.1.1 Stochastic and Diagonal Complementation

Accuracy

In this experiment we make a comparison between the accuracy achieved by our algorithm with the two types of complementation. As we stated previously, complementation is the technique that we use as way of preserving the double stochasticity of the blocks in the lower levels. In the section 2.4 we discussed about stochastic complementation of equation 2.10 and we proposed a more efficient approach, named as diagonal complementation.

¹https://sites.google.com/site/santofortunato/inthepress2
Figure 4.1: **Complementation comparison.** The plots show the accuracy of our algorithm on the second level partition after diagonal and stochastic complementation. The experiment was conducted on graphs with $N = 500$ nodes, $\mu_2 \in \{0.1, 0.2\}$ and $\mu_1$ ranging from 0.05 to 0.35. Each point is always an average over 50 realizations.

- **Stochastic Complementation.**
- **Diagonal Complementation.**
In Figure 4.1, the panels indicate the accuracy of the algorithm in detecting the second level partition of the LFR benchmark graph, as a function of the mixing parameter of the first level $\mu_1$, for two different choices of the mixing parameter of the second level $\mu_2$. The accuracy is calculated via NMI and ARI. The reason that we measure the accuracy only in the second level is because this level is affected directly by the complementation. The sub-matrices that are processed in the second level are the stochastic complements that correspond to the clusters of the first level.

The Figure 4.1 shows that diagonal complementation performs better in terms of accuracy.

**Running Time**

In this experiment we make a comparison between stochastic and diagonal complementation in terms of running time. In the Figure 4.2 somebody can see that stochastic complementation takes more running time.

**4.1.2 Cluster Determination Steps**

Recall from the Section 3.1 that the user-defined parameter repcl represents the number of iterations that our method, and specifically the Algorithm 1, needs in order to determine a cluster. In this experiment we aim at giving an insight to how to choose this parameter.
4.1. Model Parameter Tests

Figure 4.3: **Cluster determination steps.** The experiment was conducted on graphs with $N = 1000$ nodes, $\mu_1 \in \{0.05, 0.1\}$ and $\mu_2$ ranging from 0.05 to 0.2. Each point is always an average over 50 realizations.

- $\mu_2 = 0.05$
- $\mu_2 = 0.1$
- $\mu_2 = 0.15$
- $\mu_2 = 0.2$
The plots of Figure 4.3 correspond to the accuracy in the first level partition for different number of cluster determination steps (parameter `repl`). We notice that the number of iterations that are required to determine a cluster of the first level are much related to how distinct are the clusters in the second level. Specifically, the lower the values of the $\mu_2$ are (more distinct second level clusters), the more steps are required in order to determine the first level partition. This can be explained easily using the theory on stochastic dynamics of Section 2.3.

### 4.2 Quality Tests

In this part of the experimental evaluation we test the efficiency of the overall framework in terms of quality. In other words, we test how other algorithm’s results are improved by using Hsc.

We evaluated the clustering results of HSC against well known algorithms, namely SC, Ward, k-means, AL and Birch, using the well-known stand-alone quality metrics conductance, coverage and modularity (see in the beginning of the chapter for brief descriptions). We used two datasets, Ecoli and Glass. The similarity matrix for both of them was constructed as described in the Section 2.1 and depicted in the Figure 2.1. The steps we took are the following

- We obtained one level of clustering by running HSC algorithm. In both of the datasets were found two clusters in the first level.
- Then, we fed each one of the algorithms with the resulting clusters in order to find a number of further clusters (3, 4, 5 and 6).

Tables 4.2 and 4.3 show the results of the experiment, where HSC (highlighted results) outperforms clustering in most of the cases. The basic conclusion is that dividing the clustering into sub-problems in the way that we propose leads consistently to better results. The proposed framework, except for finding hierarchies of cluster has the advantage of leading to better lower level partitions, no matter what the algorithm of the second stage is.
### 4.2. Quality Tests

| Method | Clusters | Metric | conductance | coverage | modularity |
|--------|----------|--------|-------------|----------|------------|
|        |          |        |             |          |            |
|        |          |        |             |          |            |
| Sc     | 2        | 0.0285 | 0.034       | 0.9781   | 0.9744     |
|        | 3        | 0.0285 | 0.0324      | 0.948    | 0.9451     |
|        | 4        | 0.0285 | 0.0576      | 0.9089   | 0.869      |
|        | 5        | 0.0285 | 0.064       | 0.8554   | 0.7868     |
|        | 6        | 0.0285 | 0.0774      | 0.8139   | 0.721      |
| Birch  | 2        | 0.0285 | 0.0466      | 0.9781   | 0.9659     |
|        | 3        | 0.0285 | 0.0466      | 0.9123   | 0.9115     |
|        | 4        | 0.0285 | 0.0466      | 0.8875   | 0.8734     |
|        | 5        | 0.0285 | 0.0466      | 0.8476   | 0.7895     |
|        | 6        | 0.0285 | 0.0466      | 0.8433   | 0.7866     |
| Ward   | 2        | 0.0285 | 0.0466      | 0.9781   | 0.9659     |
|        | 3        | 0.0285 | 0.0466      | 0.9366   | 0.9115     |
|        | 4        | 0.0285 | 0.0466      | 0.9117   | 0.8734     |
|        | 5        | 0.0285 | 0.0466      | 0.8768   | 0.7895     |
|        | 6        | 0.0285 | 0.0466      | 0.8744   | 0.7866     |
| Al     | 2        | 0.0285 | 0.0466      | 0.9781   | 0.9659     |
|        | 3        | 0.0285 | 0.0466      | 0.9459   | 0.9017     |
|        | 4        | 0.0285 | 0.0466      | 0.9191   | 0.8963     |
|        | 5        | 0.0285 | 0.0466      | 0.9097   | 0.8603     |
|        | 6        | 0.0285 | 0.0466      | 0.9095   | 0.8182     |
| k-means| 2        | 0.0285 | 0.0398      | 0.9781   | 0.9705     |
|        | 3        | 0.0285 | 0.0374      | 0.948    | 0.9245     |
|        | 4        | 0.0285 | 0.0466      | 0.9089   | 0.863      |
|        | 5        | 0.0285 | 0.0466      | 0.8555   | 0.8395     |
|        | 6        | 0.0285 | 0.0466      | 0.8374   | 0.7348     |

**Table 4.2: Comparison on Ecoli dataset.** Shows the performance of HSC framework on several clustering algorithms for varying number of clusters. The highlighted results correspond to the result obtained by using HSC framework, while the rest correspond to the result obtained by the algorithm without the framework.
Table 4.3: Comparison on Glass dataset. Shows the performance of HSC framework on several clustering algorithms for varying number of clusters. The highlighted results correspond to the result obtained by using HSC framework, while the rest correspond to the result obtained by the algorithm without the framework.
Chapter 5

Conclusions

We presented a simple, divisive hierarchical clustering framework called Hierarchical Stochastic Clustering, that acts in two stages. In the first stage, it finds a primary hierarchy of clustering partitions in a dataset. In the second stage, it feeds a clustering algorithm with each one of the clusters of the very detailed partition, in order to settle the final result. The output is a hierarchy of clusters.

Through the experimental evaluation, we showed that our framework builds a meaningful hierarchy of clusters and improves the results of the clustering algorithm of the second stage, not only computationally, but also in terms of cluster quality. The experimental evaluation includes both synthetic graphs and real world datasets. The results suggest that HSC framework finds efficiently hierarchically nested clusters in large volumes of data.

5.1 Future Work

Some directions for future research include:

- Investigate other solutions for determining a cluster instead of looking the largest gap in the values of the vector $\pi^T$ for a predefined number of steps. In some bad conditioned scenarios this strategy leads the algorithm to form wrong clusters.

- Since we use a random seeding strategy, one future direction would be to find better seeds for minimizing both the computation time and improving the clustering determination process.

- Search for similarity measures and scaling strategies that highlight the hierarchical structure and fit to our method.
Chapter 5. Conclusions

- Examine whether we can use a few steps of Sinkhorn-Knopp scaling instead of the algorithm until it converges.
- Make a parallel implementation of the proposed framework.
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