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# Clustering and community detection in directed networks: A survey

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## ABSTRACT

Networks (or graphs) appear as dominant structures in diverse domains, including sociology, biology, neuroscience and computer science. In most of the aforementioned cases graphs are directed – in the sense that there is directionality on the edges, making the semantics of the edges nonsymmetric as the source node transmits some property to the target one but not vice versa. An interesting feature that real networks present is the clustering or community structure property, under which the graph topology is organized into modules commonly called communities or clusters. The essence here is that nodes of the same community are highly similar while on the contrary, nodes across communities present low similarity. Revealing the underlying community structure of directed complex networks has become a crucial and interdisciplinary topic with a plethora of relevant application domains. Therefore, naturally there is a recent wealth of research production in the area of mining directed graphs – with clustering being the primary method sought and the primary tool for community detection and evaluation. The goal of this paper is to offer an in-depth comparative review of the methods presented so far for clustering directed networks along with the relevant necessary methodological background and also related applications. The survey commences by offering a concise review of the fundamental concepts and methodological base on which graph clustering algorithms capitalize on. Then we present the relevant work along two orthogonal classifications. The first one is mostly concerned with the methodological principles of the clustering algorithms, while the second one approaches the methods from the viewpoint regarding the properties of a good cluster in a directed network. Further, we present methods and metrics for evaluating graph clustering results, demonstrate interesting application domains and provide promising future research directions.

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## 1. Introduction

Networks have become ubiquitous as data from many different disciplines can be naturally mapped to graph structures [1]. Technological networks, including the Internet, electrical grids, telephone networks and road networks are an important part of everyday life. Information networks, such as the hyperlink structure of the Web and citation networks, offer an effective way to represent content and information and navigate through it. Biological networks, including protein–protein interaction networks, neural networks, gene regulatory networks and food webs, can be used to model the function and interaction of natural entities. Social networks, such as collaboration networks, sexual networks and interaction networks over online social networking applications are used to represent and model the social ties among individuals. Due to the extent and the diversity of contexts in which graphs appear, the area of network analysis has become both crucial and interdisciplinary, in order to understand the features, the structure and the dynamics of these complex systems.

Real-world networks, as the ones presented above, are not classified as random networks (e.g., the Erdős–Rényi random graph model [2]); that is, they present fascinating patterns and properties conveying that their inherent structure is not governed by randomness. The degree distribution is skewed, following a power-law distribution [3,4], the average distance between nodes in the network is short (the so-called small-world phenomenon [5–7]), the ties between entities do not always represent reciprocal relations forming directed networks with nonsymmetric links [1], while edge distribution is inhomogeneous resulting in node groups with high internal edges' density and low density between them [1,8]. The last property is referred to *clustering* or *community structure* and is of great interest in various fields and real-world applications. Detecting clusters in graphs with directed edges among nodes, is the focus of this survey paper.

Informally, a *cluster* or *community* can be considered as a set of entities that are closer each other, compared to the rest of the entities in the dataset. The notion of closeness is based on a similarity measure, which is usually defined over the set of entities. In the areas of machine learning and data mining, the task of clustering is also referred as “unsupervised learning” where the aim is to group (cluster) together similar objects without any prior knowledge about the clusters (e.g., see Ref. [9]).

In the case of networks, the clustering (or community detection) problem refers to grouping nodes into clusters according to their similarity, which usually considers either topological features (e.g., features extracted from the graph), or other

characteristics related to the nodes and edges of the graph (e.g., additional information that may be associated with the nodes and edges), or both of them. In other words, the clusters typically correspond to groups of nodes sharing common properties and characteristics. Although there are several definitions for the graph clustering problem, the most common one states that a cluster corresponds to a set of nodes with more edges inside the set than to the rest of the graph.

It is important to stress out here that the task of graph clustering can be distinguished into two different problems. The first and most studied one – which is the focus of this paper – aims to group the nodes of a single graph according to some clustering definition (e.g., density). On the other hand, the second problem refers to the task where the goal is to cluster a set of graphs – treating them as individual objects – based on their similarity (e.g., see Ref. [10]).

Finding clusters in *directed networks* is a challenging task with several important applications in a wide range of domains. However, the problem of graph clustering has mainly been considered and studied for the case of undirected networks. A plethora of diverse algorithms have been proposed for the undirected settings, involving contributions from the fields of computer science, statistical physics and biology (e.g., see Ref. [11]). Nevertheless, numerous graph data in several applications are by nature directed and thus it is meaningful to incorporate all the available information during the clustering process (i.e., the directionality of the edges). Some illustrative examples include (see Section 7 for a detailed list of applications related to clustering directed networks):

- *Social and information networks*: Clusters in the directed hyperlink structure of the Web correspond to sets of web pages that share some common topics. Similarly, communities in a social network with non-symmetric links (e.g., twitter) correspond to individuals with common interests or friendship relationships.
- *Biology*: In prokaryote genome sequence data, the donor–recipient relations among genomes are modeled by directed networks (called Lateral Gene Transfer networks – LGT). Applying graph clustering methods to these directed networks enables testing hypotheses relevant to LGT patterns and mechanisms operating in nature [12].
- *Neuroscience*: Analyzing directed brain networks produced by neuron interactions, neuroscientists are able to comprehend the functional architecture of the brain [13].
- *Clustering non-graph data*: Except from the cases where the data naturally can be modeled as graphs, graph clustering algorithms can be also applied on data with no inherent graph structure, operating thus as general purpose algorithms. In such cases, the data (e.g., points in a  $d$ -dimensional Euclidean space) is represented in terms of a similarity graph corresponding to topological relationships and distance among them. Hence, the problem of clustering a set of data points is transformed to a graph clustering problem (e.g., see tutorial by von Luxburg [14]). Depending on the way the similarity graph is constructed, the final graph can contain directed edges (e.g., using  $k$ -nearest neighbor graphs or based on probabilistic dependence relations between data points [15]).

It is clearly evident that the clustering problem in directed networks is particularly significant with many important applications in several areas. Nevertheless, despite its importance, the problem has not received significant attention from the research community. Even though a plethora of directed graph data exist, the most common way to dealing with edge directionality during the clustering task, is simply to ignore it. In other words, the directed network is converted into an undirected one (by assuming edge symmetry), and then algorithms for the undirected graph clustering problem can be applied. However, in many cases, this simplistic technique would not be satisfactory, since some of the underlying semantics are not retained (e.g., in a citation network between scientific publications or in the hyperlinked structure of the Web).

The goal of this survey paper is to review the methods and algorithms proposed by the wider research community to deal with the clustering in directed networks. Some of them include extensions of approaches that have been previously applied in undirected networks while others propose novel ways as to how edge directionality can be utilized in the clustering task.

### 1.1. Challenges in clustering directed networks

The problem of clustering in directed networks is considered to be a more challenging task as compared to the undirected case. Highlighting the difficulties of the problem, in his recent work Santo Fortunato stated that “*Developing methods of community detection for directed graphs is a hard task. For instance, a directed graph is characterized by asymmetrical matrices (adjacency matrix, Laplacian, etc.), so spectral analysis is much more complex. Only a few methods can be easily extended from the undirected to the directed case. Otherwise, the problem must be formulated from scratch*” [11]. This paragraph summarized the basic challenges for the directed graph clustering problem. Moreover, the nature of relationships captured by the edges are fundamentally different from the ones in the undirected settings [16]. To this direction, we briefly discuss on some of the main challenges, which actually can be helpful to understand how the directed graph clustering is differentiated from the undirected version.

It is clear that ignoring edge directionality and considering the graph as undirected is not a meaningful way to cluster directed networks as it fails to capture the asymmetric relationships implied by the edges of a directed network. Therefore, the main challenge is to propose meaningful ways to incorporate edge directionality in the clustering process. However, even this is not sufficient. In the broader literature in graph theory and graph algorithms, the main focus is on undirected graphs. Therefore, two additional points that strengthen the challenging nature of the problem are:

- (i) While several graph concepts (e.g., density) are theoretically well founded for undirected graphs, not enough effort has been put on how to extend these concepts on directed graphs.

- (ii) Similarly, extending to the directed case the available theoretical tools that have been already applied to define and propose solutions for the undirected versions of the problem (including graph theoretic and linear algebraic tools), is not straightforward (e.g., the tool of spectral clustering based on the Laplacian matrix [17]).

In addition to the above points, a precise and common definition for the clustering problem in directed networks does not yet exist. The intuition based on the intra-cluster and inter-cluster edge density cannot be easily extended to the directed case, due to the absence of link symmetry. Moreover, the presence of directed edges implies more sophisticated types of clusters that do not exist in undirected networks and cannot be captured using only density and edge concentration characteristics (e.g., clusters that represent patterns of movement or flow circulation among nodes – see Section 3). As we will see at the rest of the paper, in the very recent literature several clustering definitions have been proposed and various algorithms have been designed to reveal different “types” of graph clusters (e.g., [18]).

## 1.2. Goals of the survey and contributions

The main goal of this survey paper is to organize, analyze and present in a unified and comparative manner the methods and algorithms proposed so far for the problem of clustering and community detection in directed networks. While a large amount of research works and related surveys have been devoted to the undirected version of the problem (see Section 1.3 for more details), our focus is on the clustering problem in the directed settings, where very recently many diverse methods and algorithms have been proposed.

Our survey adopts the following methodology:

- (i) As a first resort, we present a broad categorization of the efforts that have been proposed so far. This classification scheme is mostly concerned with the methodological principles and the algorithmic approaches for the graph clustering problem in directed networks and is mostly built upon the work for the undirected case of the problem. Hence, whenever possible we organize and review the related work describing how existing methods for undirected networks are extended in order to deal with edge directionality. Additionally, the related work is organized according to common methodological features that the approaches may share. We consider that such a classification and presentation scheme is a natural way to explore and study the relevant literature, since a large portion of the proposed approaches constitute extensions from the undirected case of the problem.
- (ii) At a second step, we present two major categories of clusters identified from the already proposed clustering methods, and then, the related work is classified to these categories. The first category corresponds to methods which adopt the more traditional density-based definition of clusters, while the second one includes methods where the extracted clusters present interesting patterns, beyond simple edge density, reflecting the existence of directed edges (e.g., flow-based patterns – Section 3).

To the best of our knowledge, this is the first comprehensive and extensive survey fully devoted to the clustering problem in directed networks. We consider that the two aforementioned axes on which the survey will align, can be helpful both for researchers in the area and for practitioners that are interested in graph clustering algorithms for directed networks (e.g., see Section 7 for some important applications where directed graph clustering methods can be applied). For the latter case, our ultimate goal is that this survey can be used as a practitioner’s guide.

## 1.3. Related surveys

There are many previous related works and surveys that refer to graph clustering and community detection in undirected networks. Fortunato [11] presents a comprehensive review in the area of community detection for undirected networks from a statistical physics perspective, while Schaeffer [19] mainly focuses on the graph clustering problem as an unsupervised learning task. Both surveys briefly discuss the case of directed networks, however their focus is on the undirected case of the problem. A similar but more compact description of clustering approaches in undirected networks is presented in Refs. [20–22]. Coscia et al. [23] present a categorization for community discovery methods according to the definition of community they adopt (e.g., communities based on internal density or bridge detection). Our work shares some common features with the one of Coscia et al. since part of our presentation follows a similar categorization scheme. Parthasarathy et al. [24] present the principal methods for the undirected community discovery problem, as well as research trends and emerging tasks in the area. One of them is community discovery in directed networks. Aggarwal and Wang [10] elaborate on the basic principles for finding communities in undirected networks, presenting some well-established approaches (e.g., spectral clustering, minimum cut problem). Moreover, a large part of their work is devoted to the problem of clustering a set of graphs, treating them as individual objects (in contrast to the node clustering problem of a single graph which is the focus of this paper). Finally, Papadopoulos et al. [25] discuss the topic of community detection in the context of Social Media.

## 1.4. Structure of the survey

The rest of the paper is organized as follows. In Section 2 we commence by providing the background and the basic terminology used throughout this survey. In Section 3 we elaborate on the problem of clustering in directed networks,

providing the basic definitions proposed in the relevant works. These clustering definitions–notions will later be used to classify the proposed methods based on the type of clusters they aim to identify. Then, in Section 4 we present the first and main methodological classification based on the algorithmic approaches they adopt to deal with edge directionality. Whenever the methods are built upon approaches for undirected networks, an incremental description is followed with respect to the undirected case. In Section 5 we present a second classification scheme of the clustering approaches according to the notion–definition of clusters in directed networks, and we also present an empirical comparison of the main methods that have been reviewed throughout this paper. In Section 6 we present the evaluation metrics for assessing the clustering results and discuss on proposed benchmarking techniques for the graph clustering task. Section 7 presents the main applications of directed graph clustering in different application domains, while in Section 8 we discuss future research directions. Finally, in Section 9 we conclude the survey by summarizing and providing remarks on the problem.

## 2. Basic terminology and background

In this section we provide the basic terminology and background that will be used throughout the paper. We give the definitions for basic graph theoretic and linear algebraic concepts, and then we describe the main aspects of random walks which play crucial role in the design of clustering and community detection algorithms. Finally, we make a brief presentation of the major metrics used to quantify the quality of a community/cluster in undirected networks. Table 1 gives a list of used symbols along with their definition. For a general introduction to the field of complex networks, the reader may refer to Refs. [26,1,27].

### 2.1. Graph theory

A *network* is usually represented by a *graph* (throughout the paper we use the terms network and graph interchangeably). A graph  $G = (V, E)$  consists of a set of nodes  $V$  and a set of edges  $E \subseteq V \times V$  which connect pairs of nodes (sometimes the nodes and edges of a graph are also called vertices and links respectively). The number of nodes in the graph is equal to  $n = |V|$  and the number of edges  $m = |E|$ . A graph may be *directed* or *undirected*, *unipartite* or *bipartite* and the edges may contain *weights* or not. Fig. 1 depicts some examples of different types of graphs.

**Definition 1** (*Directed and Undirected Graph*). In a directed graph  $G = (V, E)$ , every edge  $(i, j) \in E$  links node  $i$  to node  $j$  (ordered pair of nodes). An undirected graph  $G_U = (V, E)$  is a directed one where if edge  $(i, j) \in E$ , then edge  $(j, i) \in E$  as well.

**Definition 2** (*Bipartite Graph*). A graph  $G_B = (V_h, V_a, E_b)$  is called bipartite if the node set  $V$  can be partitioned into two disjoint sets  $V_h$  and  $V_a$ , where  $V = V_h \cup V_a$ , such that every edge  $e \in E_b$  connects a node of  $V_h$  to a node of  $V_a$ , i.e.,  $e = (i, j) \in E \Rightarrow i \in V_h$  and  $j \in V_a$ . In other words, there are no edges between nodes of the same partition.

Every graph  $G = (V, E)$  (directed or undirected, weighted or unweighted) can be represented by its *adjacency matrix*  $\mathbf{A}$ . Matrix  $\mathbf{A}$  has size  $|V| \times |V|$  (or  $n \times n$ ), where the rows and columns represent the nodes of the graph and the entries indicate the existence of edges.

**Definition 3** (*Adjacency Matrix*). The adjacency matrix  $\mathbf{A}$  of a graph  $G = (V, E)$  is an  $|V| \times |V|$  matrix, such that

$$A_{ij} = \begin{cases} w_{ij}, & \text{if } (i, j) \in E, \quad \forall i, j \in 1, \dots, |V| \\ 0, & \text{otherwise.} \end{cases}$$

The above definition is rather general and is suitable both for weighted and unweighted graphs. For the former case, each value  $w_{ij}$  represents the weight associated with the edge  $(i, j)$ , while for the latter case of unweighted graphs the weight of each edge is equal to one (i.e.,  $w_{ij} = 1, \forall (i, j) \in E$ ). If the graph is undirected, the adjacency matrix  $\mathbf{A}$  is symmetric, i.e.,  $\mathbf{A} = \mathbf{A}^T$ , while for directed graphs the adjacency matrix is nonsymmetric.

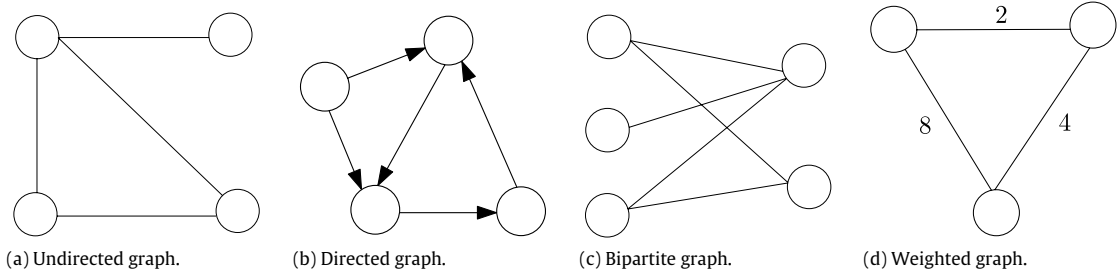
A basic property of the nodes in a graph is their *degree*. In an undirected graph  $G_U$ , a node has degree  $k$  if it has  $k$  incident edges. In the case of directed graphs, every node is associated with an *in-degree* and an *out-degree*. The in-degree  $k_i^{\text{in}}$  of node  $i \in V$  is equal to the number of incoming edges, i.e.,  $k_i^{\text{in}} = \|\{j | (j, i) \in E\}\|$ , while the out-degree  $k_i^{\text{out}}$  of node  $i \in V$  equals to the number of outgoing edges, i.e.,  $k_i^{\text{out}} = \|\{j | (i, j) \in E\}\|$ . In undirected graphs, the in-degree is equal to the out-degree, i.e.,  $k_i = k_i^{\text{in}} = k_i^{\text{out}}, \forall i \in V$ . The *degree matrix* is defined as the diagonal  $n \times n$  matrix  $\mathbf{D}$ , with the degree of each node in the main diagonal (zero entries outside main diagonal). Similarly, in directed graphs we can define the in-degree matrix  $\mathbf{D}_{\text{in}}$  and out-degree matrix  $\mathbf{D}_{\text{out}}$  for the in- and out-degrees respectively.

Let  $G_U = (V, E)$  be an undirected graph. A *path* is defined as a sequence of nodes  $v_1, v_2, \dots, v_{k-1}, v_k$ , with the property that every consecutive pair of nodes  $v_i, v_{i+1}$  in the sequence is connected by an edge. Two nodes  $i, j \in V$  are called *connected* if there is a path in  $G_U$  from node  $i$  to node  $j$ . The above definitions can be extended to directed networks, where in a *directed path*, a directed edge should exist from each node of the sequence to the next node.



**Table 1**  
Symbols and definitions.

Symbol	Definition
$G$	Directed network
$G_U$	Undirected network
$G_B = (V_h, V_a, E_b)$	Bipartite network
$V, E$	Set of nodes and edges for network $G$
$ V  = n,  E  = m$	Number of nodes and edges in the network
$e = (u, v)$	Edge $e \in E$ from node $u$ to node $v$
$\mathbf{A}_U, \mathbf{A}$	Adjacency matrix of an undirected and directed network respectively
$k_u^{\text{in}}, k_u^{\text{out}}$	In-degree and Out-degree of node $u$
$\mathbf{D}_{\text{in}}, \mathbf{D}_{\text{out}}$	Diagonal In- and Out-degree matrices
$A_{ij}$	Entry of matrix $\mathbf{A}$
$\mathbf{A}^T$	The transpose of matrix $\mathbf{A}$
$\lambda_i$	$i$ th largest eigenvalue of a matrix
$\mathbf{u}_i$	Eigenvector corresponds to $i$ th eigenvalue
$u_{ij}$	$i$ th component of $j$ th eigenvector



**Fig. 1.** Examples of different types of graphs. In the case of directed graph (b), the arrows indicate the directionality of each edge. In the weighted graph (d) the values associated with each edge represent the weights (a weighted graphs can be directed or undirected).

An undirected graph  $G_U = (V, E)$  is called *connected*, if for every pair of nodes  $i, j \in V$  a path exists from node  $i$  to node  $j$ . In the case of directed networks, three different notions of connectivity can be defined. A directed graph is called *strongly connected* if for every pair of nodes  $i, j \in V$ , there is a directed path from  $i$  to  $j$  and a directed path from  $j$  to  $i$ . A directed graph is called *connected* if for every pair of nodes  $i, j \in V$ , it contains a directed path from  $i$  to  $j$  or from  $j$  to  $i$ . Lastly, a directed graph is called *weakly connected* if ignoring the directionality of the edges (i.e., replacing the directed edges with undirected), a connected graph is produced.

A *connected component* in an undirected graph is a maximal subgraph where every pair of nodes is connected by a path. For directed graphs, the notions of *strongly connected component* and *weakly connected component* can be defined. In the former case, similar to the definition of strong connectivity that we described earlier, the edge directionality is taken into consideration, while a weakly connected component requires the existence of a path between every pair of nodes in the maximal subgraph without considering edge directionality.

## 2.2. Linear algebra and spectral graph theory

As we discussed earlier, every graph can be represented by a matrix, the so-called *adjacency matrix*. The adjacency matrix  $\mathbf{A}$  of a graph  $G = (V, E)$  is the  $|V| \times |V|$  matrix with elements  $A_{ij} = 1$  if there exist an edge between nodes  $i, j$  in the graph. In the general case where the edges of the graph contain weights, the entries of the weighted adjacency matrix correspond to edge weights. For undirected graphs, the adjacency matrix  $\mathbf{A}$  is symmetric (i.e.,  $\mathbf{A} = \mathbf{A}^T$ ), while for directed graphs the matrix is nonsymmetric.

Let  $\mathbf{A} \in \mathbb{R}^{n \times n}$  be a symmetric matrix. Then,  $\mathbf{A}$  can be written as  $\mathbf{A} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^T$ , where the orthogonal matrix  $\mathbf{U}$  contains as columns the *eigenvectors*  $u_1, u_2, \dots, u_n$  of  $\mathbf{A}$ , correspond to real *eigenvalues*  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$  and  $\mathbf{\Lambda} = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$  the diagonal matrix with the eigenvalues as entries [28–30]. The eigenvalues of the adjacency matrix define the *spectrum* of a graph and have close connections with several important graph properties. As we stated above, in the case of directed graphs the corresponding adjacency matrix is nonsymmetric and therefore the eigenvalues can be complex. Thus, it is preferable to work with the singular values of the matrix which can be extracted by the *singular value decomposition* (SVD). That is, the SVD of a real matrix  $\mathbf{A} \in \mathbb{R}^{m \times n}$  is defined as  $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$ , where  $\mathbf{U} \in \mathbb{R}^{m \times m}$  and  $\mathbf{V} \in \mathbb{R}^{n \times n}$  contain the left-singular and right-singular vectors respectively and  $\mathbf{\Sigma} = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_p) \in \mathbb{R}^{m \times n}$ ,  $p = \min\{m, n\}$ , the diagonal matrix comprised of singular values  $\sigma_i$  (note that, for symmetric matrices, the singular values correspond to the absolute values of the eigenvalues).

Another matrix commonly used to represent a graph is the *Laplacian matrix*.

**Definition 4** (*Laplacian Matrix*). In the case of undirected graphs, the Laplacian matrix is defined as

$$L_{ij} = \begin{cases} k_i, & \text{if } i = j, \\ -1, & \text{if } i \text{ and } j \text{ are adjacent,} \\ 0, & \text{otherwise,} \end{cases} \quad (1)$$

where  $k_i$  is the degree of node  $i$ . In a more compact form, the Laplacian matrix can be written as  $\mathbf{L} = \mathbf{D} - \mathbf{A}$ , where  $\mathbf{A}$  is the adjacency matrix of the graph and  $\mathbf{D} = \text{diag}(k_1, k_2, \dots, k_n)$  the diagonal degree matrix [31].

The *normalized Laplacian matrix*  $\mathbf{L}_n$  is symmetric and defined as  $\mathbf{L}_n = \mathbf{D}^{-1/2} \mathbf{L} \mathbf{D}^{-1/2}$ . In other words, if two nodes  $i, j$  are adjacent, the entry  $L_{n_{ij}}$  is equal to  $-\frac{1}{\sqrt{k_i k_j}}$ . The spectrum of the normalized Laplacian matrix  $\lambda_0 \leq \lambda_1 \leq \dots \leq \lambda_{n-1}$ , presents some interesting properties:

- All eigenvalues are non-negative. Moreover, 0 is an eigenvalue of  $\mathbf{L}_n$ .
- The number of eigenvalues with value 0 corresponds to the number of connected components in the graph.
- The smallest non-zero eigenvalue is called *spectral gap* and the corresponding eigenvector is used for the task of spectral clustering (e.g., see Ref. [14]).

A basic difference between the spectrum of the Laplacian matrix and the one of normalized Laplacian is that in the former case the eigenvalues belong to the range  $0 = \lambda_0 \leq \lambda_i \leq 2k^{\max}$ , where  $k^{\max}$  is the maximum degree in the graph, while in latter case the eigenvalues always lying in the range  $0 = \lambda_0 \leq \lambda_i \leq 2$ . For a detailed presentation of the Laplacian matrix and its properties, one can refer to the Spectral Graph Theory textbook by Chung [31].

Chung [17] defined the Laplacian matrix for directed graphs, showing interesting connections of its spectrum with the mixing rate of random walks. Very recently, Li and Zhang [32,33] proposed another generalization of the Laplacian matrix, establishing novel perspectives and results for the case of directed graphs. In Section 4.3.2 we discuss in detail about the definition of the Laplacian matrix in directed graphs and how can be used to solve the clustering problem.

### 2.3. Random walks on graphs

Generally, a random walk is a mathematical concept formalizing a procedure consisting of a sequence of random steps. In the case of graphs, given a node that corresponds to a starting point, a *random walk* is defined as the sequence of nodes formed by a repeating process starting from the initial node and randomly moving to neighborhood nodes. In other words, at each step the random walker is situated on a node of the graph and jumps to a new node selected randomly and uniformly among its neighbors.

More precisely, let  $G_U = (V, E)$  be an undirected graph and  $v_0$  be the starting node of the random walk. Let us suppose that at the  $t$ th step, the random walk is situated at node  $i$ . At  $t + 1$  step, the random walk is moving from node  $i$  to node  $j$  (neighbor of  $i$ ) with transition probability  $\frac{1}{k_i}$ . This defines the *transition matrix*  $\mathbf{P}$  of the random walk as

$$P_{ij} = \begin{cases} \frac{A_{ij}}{k_i}, & \text{if } (i, j) \in E, \\ 0, & \text{otherwise.} \end{cases} \quad (2)$$

In a compact form, this matrix can be written as  $\mathbf{P} = \mathbf{D}^{-1} \mathbf{A}$ , where  $\mathbf{D}^{-1}$  is the inverse of the diagonal degree matrix  $\mathbf{D}$ . This matrix can also be considered as a degree normalized version of the adjacency matrix. In the general case, random walks are considered to be *Markov chains*,<sup>1</sup> where the set of possible states corresponds to the vertex set of the graph.

Any distribution on a graph  $G$  can be represented by a row vector  $\boldsymbol{\pi} = [\pi_1, \dots, \pi_n]^T$ , where the  $i$ th entry captures the amount of the distribution resides at node  $i$ . In the case of random walks, the probability distribution over the graph  $G$  for each node  $i \in V$  at any time step, gives the probability of the random walk of being at node  $i$ . Thus, if  $\boldsymbol{\pi}$  is the initial distribution, then  $\boldsymbol{\pi}_1 = \boldsymbol{\pi} \mathbf{P}$  is the distribution after one step and  $\boldsymbol{\pi}_t = \boldsymbol{\pi} \mathbf{P}^t$  is the distribution after  $t$  steps. Based on the above idea, we can define a *stationary distribution*  $\boldsymbol{\pi}_s$ , as the distribution where  $\boldsymbol{\pi}_s = \boldsymbol{\pi}_s \mathbf{P}^t$ ,  $\forall t$ . In other words, the stationary distribution corresponds to a distribution that does not change over time and describes the probability that the walk is being at a specific node after a sufficiently long time. The *mixing time* is the time needed by the random walk to reach its stationary distribution. The spectrum of the transition matrix  $\mathbf{P}$  can be used to bound the mixing time of a random walk in a graph, and specifically the second largest eigenvalue [34]. In a similar manner, random walks can be defined over directed graphs. However, in this case, two main difficulties can occur: (i) at some time point, the random walker can be situated in a node with no outgoing edges, and (ii) nodes with no incoming edges will never be reached. As we will present later, the PageRank algorithm is a random walk process on directed graphs that overcomes the above problems [35].

The theoretical tool of random walks is closely related to the problem of clustering and community detection in graphs (e.g., Ref. [36]). For example, it is known that matrix  $\mathbf{P}$  has always the largest eigenvalue equal to one. In the case of networks with very clear community structure, matrix  $\mathbf{P}$  will also have  $c - 1$  eigenvalues close to one, where  $c$  is the number of well-defined modules (clusters) in the network; the rest of the eigenvalues will be relatively away from one. The eigenvectors

<sup>1</sup> Wikipedia's lemma for Markov chain: [http://en.wikipedia.org/wiki/Markov\\_chain](http://en.wikipedia.org/wiki/Markov_chain).

correspond to the first eigenvalues can be used to extract the clustering structure: for nodes that belong on the same clusters, their components in the eigenvectors will have similar values, following a step-wise form. The number of steps, corresponds to the number of clusters  $c$ . In Section 4.3.3 we provide more details on this issue and we present random walk based techniques for the case of directed networks. For a more detailed discussion on various aspects of random walks, the reader can refer to Refs. [37,31].

## 2.4. Quality measures

As we have already mentioned, a cluster or community in a network is typically considered as a group of nodes with better connectivity (and/or stronger interactions) among its members than with the nodes of different communities. Usually, the process of detecting communities in networks follows a two step approach:

- (i) First, a quality measure (or objective function) needs to be specified, that captures the notion of community structure as groups of nodes with better internal connectivity than external (or more generally, an objective criterion which quantifies the desired properties of a community).
- (ii) Then, using algorithmic techniques, the nodes of the network are assigned to specific communities, optimizing the objective function. Since the optimization process of the objective functions typically leads to computational difficult problems (e.g., see Ref. [19]), a common approach is to employ heuristics or other approximation techniques.

In the literature several measures have been proposed for quantifying the quality of communities in networks (most of them have been introduced for the case of undirected networks, but some of them have been also extended to directed ones; in Section 4.3 we describe some of these measures in detail and we also present their extensions to directed networks). Typically, some of the quality measures focus on both the intra-cluster and inter-cluster edge density (*multi-criterion* scores), such as normalized cuts [38], conductance and expansion. Other measures focus only in one of them (*single-criterion* scores) and a well-known representative of this category is modularity (e.g., see Refs. [11,19,39] for a recent comparative study of quality measures in undirected large scale networks).

*Modularity* [40,41] is one of the most popular and widely used metrics to evaluate the quality of network's partition into communities. Considering a specific partition of the network into clusters, modularity measures the number of edges that lie within a cluster compared to the expected number of edges of a null graph (or configuration model), i.e., a random graph with the same degree distribution. In other words, the measure of modularity is built upon the idea that random graphs are not expected to present inherent community structure; thus, comparing the observed density of a subgraph with the expected density of the same subgraph in case where edges are placed randomly, leads to a method for identifying clusters. More precisely, the modularity value  $Q_u$  of a specific partition of an undirected network into communities is defined as follows

$$Q_u = \frac{1}{2m} \sum_{i,j} \left[ A_{ij} - \frac{k_i k_j}{2m} \right] \delta(c_i, c_j), \quad (3)$$

where  $\mathbf{A}$  is the adjacency matrix,  $c_i, \forall i \in V$  is the community membership of node  $i$  and  $\delta(c_i, c_j) = 1$  if  $c_i = c_j$  (i.e., if nodes  $i, j$  belong to the same community) and 0 otherwise. The modularity value can be either positive or negative. Higher positive values indicate better community structure properties and therefore, finding the partition that maximizes the modularity provides a method for extracting the underlying community structure. More details on modularity as well as its extension to directed networks are presented in Section 4.3.1.

Optimizing the modularity function is a computational difficult task [42]; however several heuristics and approximation techniques have been proposed. Newman [43] proposed a greedy search algorithm for the problem of modularity maximization. Initially, every node of the graph belongs on its own community; then, iteratively, pairs of communities are joined on the same group if they achieve the highest increase of the modularity value. Thus, the algorithm can be considered as an agglomerative hierarchical clustering method (e.g., see Ref. [9]) and the whole procedure can be represented by a dendrogram. Clauset et al. [44] presented a faster greedy algorithm (almost linear time in sparse graphs), based again on an hierarchical clustering approach. Other well known methods for modularity optimization are the ones rely on spectral techniques. For example, Newman [41] showed that the measure of modularity can be expressed in terms of the spectrum of a specific matrix associated to the network (called *modularity matrix*), and therefore spectral techniques can be applied in the optimization process. In Section 4.3.1 we present a similar approach for the case of directed networks. Other methods apply simulated annealing techniques [45] (e.g., Refs. [46,47]) and extremal optimization [48]. For a more detailed presentation of modularity optimization techniques, the reader can refer to the survey paper of Fortunato [11]. Similar optimization approaches can be also applied to directed networks.

However, as noted by Fortunato and Barthélemy [49], modularity suffers from the so-called *resolution limit*. That is, modularity optimization may fail to detect communities with size smaller than a scale which mainly depends on the size of the network. This point is particularly significant since typically real world networks contain communities of various sizes.

## 3. Clusters in directed networks – intuition and discussion

In this section we introduce the notion of clusters or communities in directed networks and we discuss about their structural properties. We provide different intuitive definitions regarding the properties of clusters, that will enable the



reader to better comprehend the notion of clustering in directed networks and subsequently to classify the clustering methods according to the definition given. It is important to stress out here that there is no well defined definition for the graph clustering problem, both in the directed and undirected cases. Actually the formulation depends either on the application domain or generally on the type of clusters we are interesting in. Nevertheless, regardless of the problem definition, the ultimate goal of the clustering task remains the same: the graph nodes should be assigned to clusters, with “similar” nodes belonging to the same cluster.

Let us now present a high level definition of a cluster or community in networks which can be considered as a generic definition for the clustering task. Later, we capitalize on this to capture and describe different possible clustering structures for directed networks, as they have been proposed in the literature.

**Definition 5** (*High Level Definition of a Cluster*). A cluster or community in a network can be considered as a set of nodes that share common or similar features (characteristics).

In this generic definition, there are two things that need to be specified: (a) the notion of similarity among the nodes of a directed network and (b) the features/characteristics we are interesting in. We consider that specifying these two elements, we are able to capture and describe all possible clustering notions in directed networks. In order to become more precise, let us consider as example the traditional definition of clusters as modules with dense connections between the nodes of the same cluster but sparser connections between different clusters [41,50]. According to the above definition, the features correspond to graph's edges, while the number of edges between a set of nodes (density) can be considered as a similarity node indicator in the graph.

Having defined the desired properties of the clustering structure, then the process of detecting communities is a two step approach: first, we should specify an objective function that captures the notion of clustering structure, according to the chosen definition. Then, using algorithmic techniques, the nodes of the network are assigned to specific clusters, optimizing the objective function. In Section 2, we gave a brief introduction about objective functions for undirected networks. Later at this paper, we will describe such objective criteria for directed networks, as well as approaches for detecting the community structure.

Next, we present the two main notions—definitions (or categories) for clusters in directed networks:

- (a) *Density-based* clusters, i.e., groups of nodes that follow the traditional clustering definition based on edge density characteristics.
- (b) *Pattern-based* clusters, i.e., groups of nodes that go beyond edge density patterns. As we will describe shortly, an example of this category is the case of flow circulation, where a pattern of movement induced within the nodes of the cluster.

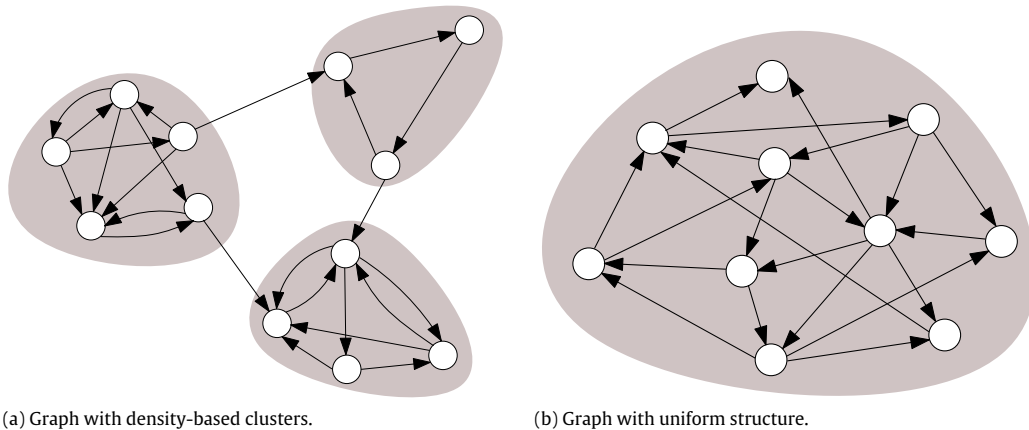
This classification can also be extended to undirected networks, as some research works propose [23,51,52]). Then the question rising is: which clustering definition for directed networks should one adopt? The answer highly depends on the application domain and on the features of the network dataset under consideration. Such features may include the nature of interactions among graph's nodes (as captured by the edges) and prior knowledge of the underlying structure. In Section 7 we present a list with real applications of directed graph clustering, along with the most suitable clustering definition.

### 3.1. Density-based clusters

We consider *density-based clusters*, that can be regarded as the more traditional definition of communities/clusters in both directed and undirected networks, and also the most well studied in the research community (e.g., Refs. [40,8,41,50]). The notion of density-based clusters is entirely based on the distribution and topology of the edges inside the network. As we mentioned earlier, according to this definition, a cluster in directed networks is defined as a group of nodes with more intra-cluster than inter-cluster edges. Fig. 2(a) depicts an example of a directed network which contains three well defined density-based clusters. It is clear that the edge density within each cluster (shadowed regions) is much larger than the density between different clusters. On the other hand, Fig. 2(b) presents a homogeneous directed network with uniform edge distribution among nodes. The network lacks a modular organization and thus there is no obvious density-based community structure. Based on this definition, the goal of a graph clustering algorithm is to assign the nodes into clusters, maximizing the number of edges within clusters, while minimizing the inter-cluster edges. As we will see later, there are several popular density-based graph clustering techniques, that either trying to maximize the internal cluster density, either minimize the number of extra-cluster edges or both of them.

The above notion of clustering in directed networks can be considered as a natural extension from the graph clustering problem in undirected networks (e.g., Refs. [40,11,19,23]). In the next sections of the paper we will see that some techniques, initially introduced for undirected networks, form the basis for dealing with the directed graph clustering problem.

Moreover, for the undirected case, the density-based definition has close connections with the well-known *graph partitioning* problem in the field of computer science (e.g., Ref. [53]). However, there are two main differences between them: (a) in the graph partitioning problem, the desired number of partitions (or clusters)  $k$  is a parameter of the problem and needs to be specified a priori, while in the case of graph clustering and community detection problems this is not always prerequisite, and (b) the goal of the partitioning problem is to equally assign nodes in the different partitions, where the size of each cluster will be approximately equal to  $\frac{n}{k}$  [11]. On the other hand, in the clustering problem, the distribution of the clusters' sizes may not be uniform.



**Fig. 2.** Two directed graph examples. The left one (a) consists of three density-based clusters, while the right one shows a homogeneous link density with the absence of obvious community structure.

It is important to note here that extending the notion of density-based clusters to directed networks is not always a trivial procedure. While some of the proposed objective measures for the undirected case can be easily extended to directed graphs by considering in a meaningful way the directionality of the edges (e.g., the criterion of modularity [50]), due to the existence of directed edges, some of the desired cluster properties may not hold. Even worse, some graph-theoretic measures and concepts that help us to evaluate the quality of density-based clusters cannot be easily extended and defined in the directed case. For example, as pointed out by Schaeffer [19], each cluster in a graph should be *connected* (i.e., there should be at least one path between every pair of nodes in the graph). As mentioned in Section 2, in directed graphs, the connectivity property can be expressed in three forms: weak connectivity, connectivity and strong connectivity. Depending on the required cluster properties, any of the above criteria can be adopted in the definition of density-based clusters for directed networks. This is just an indication where simple graph concepts, such as connectivity, become complex when edge directionality is taken into consideration.

### 3.2. Pattern-based clusters

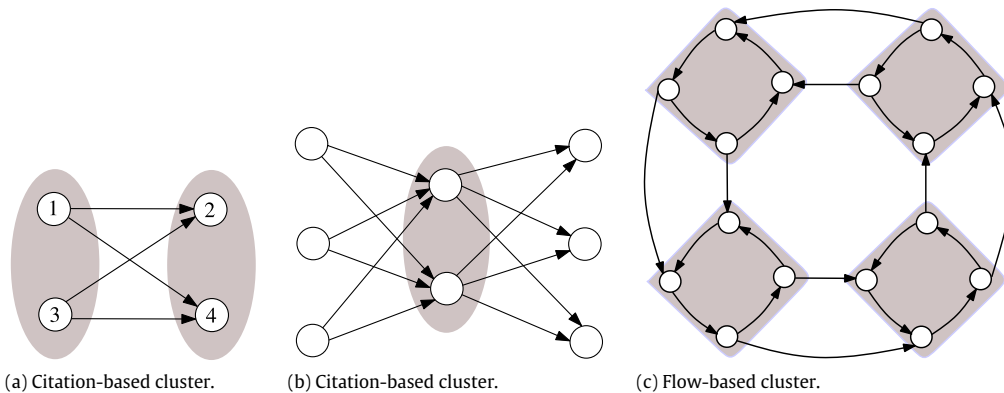
Previously we presented the notion of density-based clusters that constitute the major type of clustering structure in directed networks. Although this represents the most common and well-studied clustering definition in both directed and undirected networks, it cannot capture more sophisticated clustering structures, than the classical well-cohesive groups, where edge density may not represent the major clustering criterion. More precisely, the nodes of a directed network can be naturally clustered together according to similar connectivity patterns that may exist and are not captured completely applying only density criteria. Actually, in some cases, two or more nodes can belong to the same cluster even though they are not directly connected by common edges. We refer to this category of clusters as *pattern-based clusters*, since they represent structures with interesting connectivity properties in directed networks.<sup>2</sup>

Examples of patterns that are interesting for clustering directed graphs are the cases of co-citation and flow. Co-citation implies that a set of nodes  $A$  links to a set of nodes  $B$  and this structure implies a similarity among the members of each group – i.e., the members of  $A$  are similar among them as they all point to the same nodes, group  $B$ . Another interesting pattern has to do with the network flow at the cluster level, i.e., the linking structure within a cluster forces that the flow through the links predominantly stays within the cluster instead of pouring out of it.

Fig. 3 depicts three cases of graphs that contain different types of pattern-based clusters (as shown in the shadowed regions). The first graph (a) forms two clusters – we will refer on them as citation-based clusters. The most interesting point in this case is that the nodes of the graph that are clustered together do not have an edge between them. Their similarity emanates from the co-citation event – i.e., the nodes of the leftmost cluster point to the nodes of the right cluster. Respectively the two nodes of the right cluster are pointed by the same group of nodes. This is actually a bipartite graph where the partitions represent two different communities. For example, let us consider the case of a citation network where nodes correspond to scientific papers and a directed edge from paper 1 to paper 2 implies that the first paper cites the latter. Although papers 1 and 3 do not share an edge, they form a natural cluster since they both cite papers 2 and 4 and it is probable that they belong on the same scientific topic.

A similar example of pattern-based clusters, appears in Fig. 3(b). In this case the two nodes in the shadowed region form a cluster, since they have out-links to the same nodes, while at the same time having in-links from the same group

<sup>2</sup> In the case of undirected networks, similar terms and definitions have been proposed for characterizing clusters with interesting connectedness patterns (e.g., Refs. [51,52,23]). Here, we extend this notion by considering clustering types that inherently arise in several real-world directed networks due to the existence of non-reciprocal relationships.



**Fig. 3.** Different examples of pattern-based clusters in directed networks. The leftmost network (a) and the one in the center (b) represent citation-based clusters. The graph on the right (c) depicts a graph with four flow-based clusters.  
Source: Figures redesigned from Refs. [54,18].

of nodes. This structure constitutes a common situation in the context of directed graphs. For example, these two nodes may correspond to the websites of two competing companies of the same market sector; they both link and are linked by a common group of webpages, but actually they do not have links among them due to competition [54]. According to our high level definition of clusters in directed networks (Definition 5), in this case the clustering features correspond to the common neighbors in the graph and thus the nodes are clustered together if they share common neighbors.

A different case of pattern-based clusters is the one presented in Fig. 3(c). The main characteristic of this network is that the edges form patterns of flow among nodes. In other words, the local interactions in the network combined with the edge directionality, induce a flow of information among the entities and therefore the clustering structure depends on how information flows (see Ref. [18] by Rosvall and Bergstrom). Then, a cluster or community in the network corresponds to a group of nodes where the flow is larger (more persistent) as compared to the flow outside the group. Assuming a user that conducts random walk on the graph, a flow-based community is a group of nodes where a random surfer is more likely to be trapped inside instead of moving out of the group [55,56].

*Remark* We should note here that both types of clusters – co-citation and flow based ones – may co-exist in a directed network. For example, as we can see from the related literature, most of the techniques that adopt the citation-based clustering rule, are also able to identify density-based clusters. However, the novelty of these techniques resides exactly on this point; through appropriate transformations, a density-based technique can be enhanced with pattern-based clustering features.

#### 4. Dealing with edge directionality: approaches for identifying clusters-communities in directed networks

There have been different directed network clustering approaches depending on the way directed edges are treated. In this section we review the clustering methods based on the methodological principles and algorithmic approaches followed. To the best of our knowledge this is the first proposal for a classification scheme of graph clustering methods for directed networks.

Since a large amount of work for the graph clustering problem in directed networks is built upon clustering approaches for undirected ones, whenever necessary we review the basic concepts to make our presentation self-contained. We also consider that giving meaningful connections to the undirected case will be helpful to the reader. For a detailed description of the undirected graph clustering methods, the reader may refer to previous interesting surveys in the field (see Section 1.3).

The proposed classification follows:

- *Naive graph transformation approach:* In this class we classify algorithms that ignore edge directionality and treat graph as undirected. Thus, clustering algorithms that have been proposed for undirected networks can be also applied to reveal the underlying community structure of directed ones (e.g., see Section 1.3). However, due to naive graph conversion, the underlying graph semantics are not retained and useful information is not taken into consideration during the clustering task. For instance, consider a citation network, where papers are represented by nodes and edges are the citations. Then assume a paper  $i$  cites paper  $j$  but not vice versa. Using the naive graph transformation each directed edge is replaced by an undirected one; thus a reciprocal relationship is introduced among papers  $i$  and  $j$  which misses to represent the endorsement of paper  $i$  to paper  $j$ .
- *Transformations maintaining directionality:* In this class we have methods where the directed graph is converted into an undirected one, either unipartite or bipartite, and edge direction is meaningfully maintained in the produced network. For example, in some approaches the directed network is converted into an undirected and weighted one, where information about directionality is introduced via weights on the edges of the graph (e.g., Ref. [54]). Then, algorithms and tools for

clustering undirected weighted graphs can be applied. In other approaches, the directed network is converted into a bipartite one and then appropriate clustering algorithms are applied to the bipartite graph (e.g., Ref. [57]).

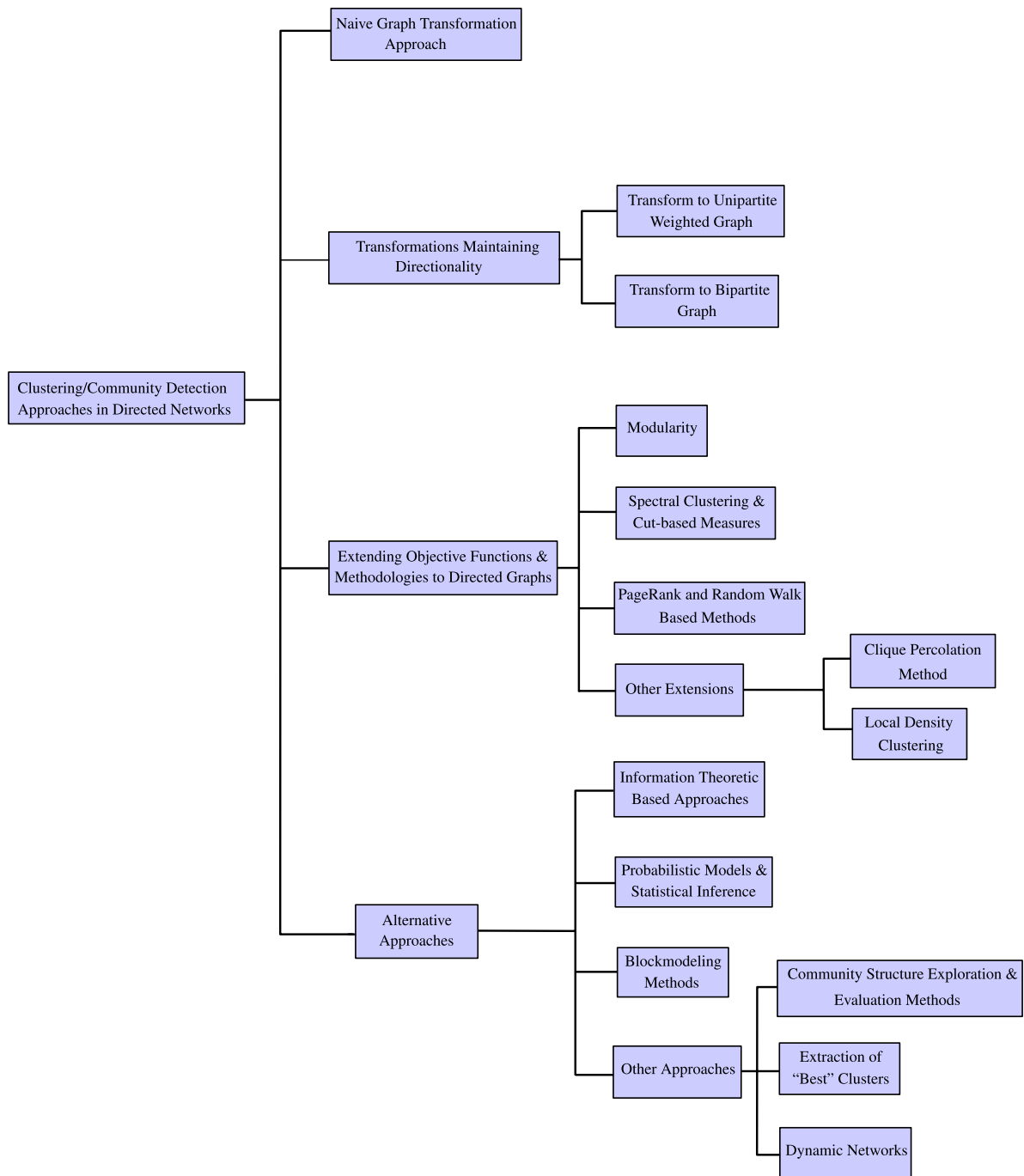
- *Extending clustering objective functions and methodologies to directed networks:* This category includes approaches that constitute extensions of methodologies from the undirected case. Thus objective criteria are extended to meet the requirements of the problem. The graph clustering problem is typically expressed as an optimization problem, where an objective criterion, capturing the desired cluster properties, is optimized by re-assigning nodes into clusters. The algorithm iterates usually until a local min/max value is reached. Since most of the research literature has focused on the undirected version of problem, a large bulk of interesting approaches regarding the properties and functionality of the (undirected) objective criteria have been presented (e.g., modularity [40,41] and normalized cut [38]). Hence, a natural way to deal with the directed version of the graph clustering problem is to extend these measures for directed networks, where edge directionality is considered as an inherent network characteristic. Some prominent representatives of this category are the directed versions of modularity [50,55,58] and the objective function of weighted cuts in directed graphs [59]. Similarly, another well established approach in this direction is the extension of algorithmic tools that have been introduced for undirected graphs. One of the most well-known such approaches is the case of spectral graph clustering based on the Laplacian matrix [14,60]. While Laplacian based spectral clustering methods initially applied on undirected networks, recent advances in the field make them also applicable to directed ones (e.g., Refs. [17,61]).
- *Alternative approaches:* This category includes approaches that follow diverse methodologies, mainly different from the ones described in the previous three categories. We identify three major types of methods, namely (i) information-theoretic, (ii) methods based on probabilistic models and statistical inference, and (iii) stochastic blockmodeling methods. Even though the last two methodologies are closely related and both refer to probabilistic models, we review them independently since they rely on different statistical inference concepts. Furthermore, in this category we also review several additional approaches that mostly concern some variations of the community detection problem in directed networks. Some of these pose interesting features and may constitute interesting extensions for future research work in the field (e.g., community detection in dynamic directed networks).

Next we will elaborate on each of the above categories with more details, presenting their basic points and classifying the related works. This is the main proposed classification scheme for the clustering problem in directed networks. Fig. 4 depicts schematically the proposed taxonomy of the different approaches for the problem. A large amount of research work has been devoted to methods that belong on the third category (extending methodologies to directed networks). We also note here that, some of the approaches share diverse methodological features (e.g., methods that transform the graph to undirected but at the same time propose extensions for the modularity objective criterion that is in accordance with their framework). Then, we do not assign them crisply in only one category; whenever necessary, we follow an overlapping classification trying to capture and present the features of each approach from all possible viewpoints. Lastly, we will shortly discuss why the naive approach is not appropriate for dealing with directed networks.

#### 4.1. Naive graph transformation approach

The first and simplest approach for the clustering problem in directed networks, is to discard edge directionality and treat graphs as undirected. After this simple transformation step, a large bulk of methods that have been proposed for undirected networks can be applied to extract the community structure (e.g., see Section 1.3 for details). Even though this is a common way in the related literature to deal with directed networks, this approach has several drawbacks that mainly derive from the fact that the information represented by edges' direction is ignored and not utilized during the clustering process. In other words, directed edges typically indicate the existence of nonreciprocal relationships between entities represented by the nodes of the graph, and thus a naive transformation to an undirected graph with symmetric relationships does not retain the underlying semantics. The two main drawbacks of this approach can be summarized as follows:

- Data ambiguities:* the naive graph transformation introduce ambiguities and to some degree incorrect information in the network. For example, let us consider the case of a citation network where a directed edge  $(i, j)$  represents a citation from paper  $i$  to  $j$ . Converting this edge into an undirected one implies a mutual relation, i.e. an edge  $(j, i)$  that does not exist in the graph. But more generally, even if someone argue that the new undirected edge represents similarity among papers  $i$  and  $j$  (since the first one cites the second), this does not always hold for both directions (i.e., paper  $j$  may be an important paper, but in a different area; thus mutual relationship and similarity may not exist). Similar concerns could be used to justify possible ambiguities introduced by this transformation approach in other domains.
- Deviations in clustering results:* even if one could ignore the ambiguities introduced in the data by the naive graph transformation approach, these may have impact to the final outcome of a clustering algorithm. Discarding edge directionality, valuable information is not utilized at the clustering process, which at the end leads to deviations at the results. In other words, clusters that exist in the initial directed network may not be identified at the transformed one, due to the naive graph conversion process. This mainly occurs because the existence of directed edges forms interesting structural patterns and clusters (e.g., the flow-based clusters that we described in Section 3.2) that cannot be found in undirected networks. Of course, this is something closely related to the definition/notion of a cluster; nevertheless, even for the same clustering definition, the approach may lead to different results at the end. Fig. 5 depicts an example of a directed graph, where a naive transformation could distort the clustering results.



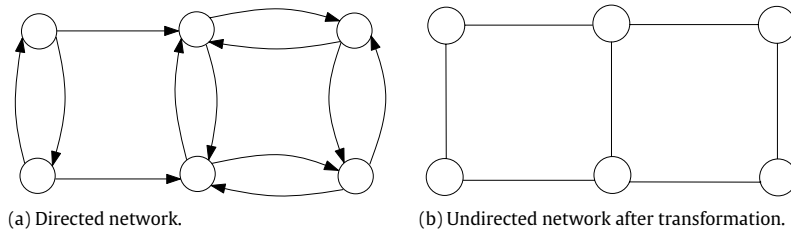
**Fig. 4.** The proposed taxonomy of clustering/community detection approaches in directed networks.

It becomes clear that this approach is not effective and could possibly lead to incorrect inference about the underlying community structure. In the following section, we will describe more meaningful graph transformation approaches, where information about edge directionality is incorporated in the final network and utilized properly during the clustering process.

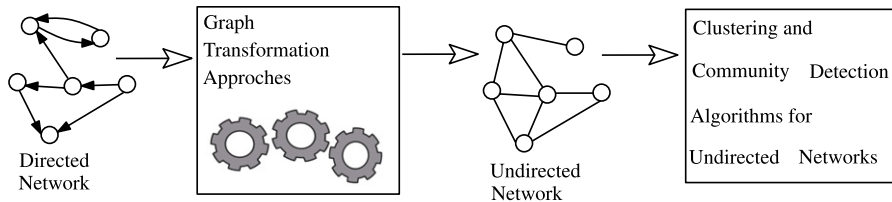
#### 4.2. Transformations maintaining directionality

In this section we will review the second category of approaches for the clustering problem in directed networks. More precisely, we will present methods that perform “meaningful” transformations of the directed network into an undirected





**Fig. 5.** Example of a naive graph transformation. The directed network (a) contains two communities, since the two leftmost nodes are connected to the rest of the network but only in one direction. After a naive graph transformation (b) it is difficult to identify any community structure.



**Fig. 6.** Schematic representation of transformations that maintain directionality: the directed network is transformed to undirected (weighted or unweighted, unipartite or bipartite) based on specific methodologies. Then, any clustering algorithm for undirected networks can be applied. The extracted clusters correspond to the clusters of the initial directed network.

one, where the term meaningful is used to denote the difference to the previously described naive transformation method. According to this approach, the basic components of the clustering task in directed networks can be summarized as follows:

1. Transform the directed network to undirected.
2. Edges' direction information should be retained as much as possible (e.g., by introducing weights on the edges of the transformed network).
3. Apply already proposed clustering algorithms designed for undirected networks.
4. The extracted communities will also correspond to the communities of the initial directed network.

More precisely, the initial graph is transformed into an undirected one, while information and semantics about the direction of the edges is meaningfully incorporated in the resulting graph. For example, this can be done by adding weights on the edges of the transformed network (or applying a reweighting scheme in case of already weighted networks). The resulting network can be either unipartite or bipartite. Then, algorithms that work on undirected networks can be applied to detect the community structure; such approaches can benefit from the plethora of diverse algorithms that have been proposed for the community detection task in undirected networks. Schematically, a high level description of this approach is depicted in Fig. 6.

#### 4.2.1. Transformation to unipartite weighted network

In a commonly used transformation approach in the related literature, the directed network is converted into an undirected unipartite one, where information about directionality is incorporated via weights on the edges of the transformed network. Satuluri and Parthasarathy [54], investigate how the problem of clustering directed graphs can benefit using such symmetrization approaches. The basic insight on their approach is that, in directed networks, a meaningful cluster can be a group of nodes that share similar incoming and outgoing edges. In other words, a clustering approach should not be based solely on density criteria, but also the in-link and out-link node similarity should be taken into consideration. Therefore, their approach is able to detect groups of nodes with homogeneous in-link and out-link structure (e.g., citation-based clusters), that do not necessarily share edges among them (e.g., similar to the clusters in Fig. 3(b)). More precisely, the authors propose a two-stage framework which is in accordance with the above discussion: (a) transformation to undirected graph applying symmetrization methods to the adjacency matrix and (b) clustering the symmetrized graph using existing algorithms. Let  $G$  be the initial directed graph with adjacency matrix  $\mathbf{A}$ . The authors discuss and propose various ways to symmetrize a directed network:

- **$\mathbf{A} + \mathbf{A}^T$  symmetrization:** In this approach, the produced undirected network  $G_U$  will have the symmetric adjacency matrix  $\mathbf{A}_U = \mathbf{A} + \mathbf{A}^T$ . The network retains the same number of edges (i.e., every directed edge is replaced by an undirected), but in the case of directed edges in both directions, the weight of the new edge is the sum of the weights in the initial directed edges. However, this simple way to symmetrize a directed network cannot capture the notion of node similarity based on incoming and outgoing edges; although the two central nodes of Fig. 3(b) exhibit structural similarity according to their in-links and out-links, they continue to remain unconnected at the resulting graph, and therefore, it is very difficult to be clustered together.

- *Symmetrization based on random walks*: according to this approach, the normalized cut (Ref. [38]) of a group of nodes in the produced undirected network  $G_U$  will be preserved with respect to the initial directed one. In other words, the directed normalized cut of a group of nodes will be equal to the normalized cut of the same group in the symmetrized undirected network. More precisely, the transformed graph will be described by the following adjacency matrix

$$\mathbf{A}_U = \frac{\mathbf{\Pi P} + \mathbf{P}^T \mathbf{\Pi}}{2}, \quad (4)$$

where  $\mathbf{P}$  is the transition matrix of the random walk and  $\mathbf{\Pi} = \text{diag}(\pi_1, \pi_2, \dots, \pi_n)$  is the diagonal matrix with the probabilities of staying at each node in the stationary state (stationary distribution). As noted by the authors (Ref. [54]), this approach makes easier the extraction of clusters that satisfy the criterion of low normalized cuts, since this property is preserved during the symmetrization process (compared to approaches that will be presented later at this papers and rely on expensive spectral clustering based on the directed Laplacian matrix (see Section 4.3.2)). However, the symmetrization method follows the density-based clustering notion due to the dependence to the normalized cut criterion, and therefore other types of meaningful structures like the case of pattern-based clusters of Fig. 3(b) with low normalized cut, cannot be easily identified.

- *Bibliometric symmetrization*: both previous approaches maintain intact the edge set of the directed network (discarding directions); they only reweight them according the selected symmetrization scheme. However, a natural requirement that a symmetrization approach should meet is that at the final graph, edges should appear between similar nodes even though in the original network this does not happen. The prime example for this argument is the network of Fig. 3(b), where there exist nodes that do not share common edges, but both of them point to the same group of nodes (and pointed by the same group of nodes). Therefore, these nodes share an intuitive notion of similarity and thus a clustering algorithm should be able to group them together.

The authors of Ref. [54] propose a symmetrization approach based on a combination of the bibliographic coupling matrix  $\mathbf{B} = \mathbf{A}\mathbf{A}^T$  and the co-citation strength matrix  $\mathbf{C} = \mathbf{A}^T \mathbf{A}$ . Both these matrices are symmetric. The former captures common outgoing edges between each pair of nodes (i.e., the number of common nodes that both nodes point to), while the latter common incoming edges (i.e., the number of nodes that commonly point to these nodes). These matrices were first introduced in the field of bibliometrics, but later have been used in several applications and domains where symmetric matrices are required (e.g., information retrieval [62] and network analysis [63]). Since both incoming and outgoing edges should be of the same importance for a clustering algorithm, the authors propose to use the sum of these matrices as a symmetrization scheme:

$$\mathbf{A}_U = \mathbf{A}\mathbf{A}^T + \mathbf{A}^T \mathbf{A}. \quad (5)$$

- *Degree-discounted symmetrization*: one of the main properties of real-world networks is that they follow a power-law degree distribution (e.g., Ref. [4]). The property states that, inside the network, there exist a few nodes with very high degree compared to the majority of the nodes. This observation has direct implications to the previously described symmetrizations, since nodes with high degree would be shared a lot of common edges with other nodes (and thus higher similarity). To this direction, the authors propose a symmetrization approach where the contribution of each node to the similarity score will be normalized according to its degree (in-degree and out-degree respectively). More precisely, their approach is based on two intuitive observations:

Case 1: Suppose that two nodes  $i, j$  both point to a node  $z$ , which has high in-degree  $k_z^{\text{in}}$ .

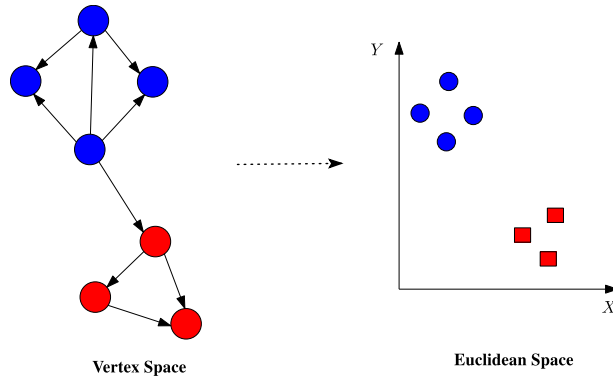
Case 2: Suppose that two nodes  $i, j$  both point to a node  $z$ , with low in-degree  $k_z^{\text{in}}$  (i.e., it has incoming edges from only a few nodes other than  $i, j$ ).

Based on these two points, the authors suggest that Case 2 should contribute more to the similarity between nodes  $i, j$  since it is a less frequent event and thus more informative. Hence, when two nodes  $i, j$  both point to a third one  $z$ , the similarity between them should be inversely proportional to the in-degree  $k_z^{\text{in}}$  of node  $z$ . Similarly, the number of outgoing links of the nodes should be taken into consideration. Thus, the out-link similarity between  $i, j$  should be inversely related to the out-degrees of nodes  $i$  and  $j$ . Then, both the bibliographic coupling and co-citations matrices (matrices  $\mathbf{B}$  and  $\mathbf{C}$  respectively) are redefined according to the degree-discounted idea as follows:

$$\mathbf{B} = \mathbf{D}_{\text{out}}^{-\alpha} \mathbf{A} \mathbf{D}_{\text{in}}^{-\beta} \mathbf{A}^T \mathbf{D}_{\text{out}}^{-\alpha} \quad \text{and} \quad \mathbf{C} = \mathbf{D}_{\text{in}}^{-\beta} \mathbf{A}^T \mathbf{D}_{\text{out}}^{-\alpha} \mathbf{A} \mathbf{D}_{\text{in}}^{-\beta}, \quad (6)$$

where  $\alpha, \beta$  are the discounting parameters. Finally, the produced similarity matrix (and thus the adjacency matrix of the symmetrized undirected network) will be the sum of these two matrices,  $\mathbf{A}_U = \mathbf{B} + \mathbf{C}$ . The authors report that they have empirically observed that setting  $\alpha = \beta = 0.5$  results into intuitive and meaningful clusterings. Having now symmetrized the directed network, algorithms designed to work on undirected graphs can be applied to extract the underlying community structure.

In a similar spirit, Lai et al. [56] proposed a symmetrization method based on network embeddings, that indirectly can be considered as a transformation to an undirected weighted network. More precisely, the basic idea is to embed the initial directed network into a vector space, preserving as much as possible from its local topological characteristics. According to this approach, every node in the directed network can be treated as a point in the Euclidean space, as schematically shown in Fig. 7.



**Fig. 7.** Visual representation of the network embedding method by Lai et al. [56]. Each node in the directed network is treated as a point in the Euclidean space (or similarly as a vector). The local topological characteristics of each node should be preserved by the embedding.

Source: Figure redesigned from Ref. [56].

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This can be considered as an equivalent representation scheme for a network, since in the general case, the adjacency matrix can be treated equivalently as a representation in a Euclidean vector space and more precisely in the space defined by the nodes of the network, that is  $\mathbb{R}^n$ . Essentially the authors rely on a specific type of network embedding and in particular on the Laplacian embedding for directed networks. As we described in Section 2, the Laplacian matrix is an alternative matrix representation for a network with several interesting characteristics. Similar to the adjacency matrix, the Laplacian can be considered as a network representation in the Euclidean space, where the similarities among node pairs are preserved. The authors are based on the extension of Laplacian matrix for directed networks proposed by Chung [17] (see Section 4.3.2 for more details on the Laplacian matrix)

$$\mathbf{L} = \mathbf{\Pi} - \frac{\mathbf{\Pi}\mathbf{P} + \mathbf{P}^T\mathbf{\Pi}}{2}, \quad (7)$$

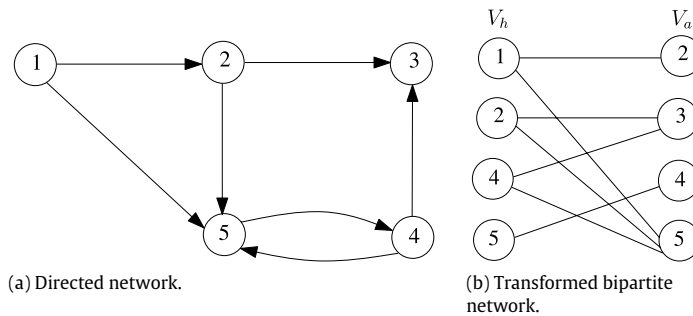
where  $\mathbf{P}$  is the transition matrix of the random walk and  $\mathbf{\Pi} = \text{diag}(\pi_1, \pi_2, \dots, \pi_n)$  the diagonal matrix with the probability of staying on each node in the stationary state.

The idea is similar to the random walk symmetrization presented earlier as again the same concept is utilized in order to define the Laplacian matrix (in this case, the PageRank random walk). However, the authors observed that the directed version of the Laplacian matrix in Eq. (7) can be expressed as  $\mathbf{L} = \mathbf{\Pi} - \mathbf{W}$ , where  $\mathbf{W} = \frac{\mathbf{\Pi}\mathbf{P} + \mathbf{P}^T\mathbf{\Pi}}{2}$ . Matrix  $\mathbf{W}$  is symmetric, while  $\mathbf{\Pi}$  can be considered as the degree matrix of the network. Hence,  $\mathbf{W}$  can be interpreted as the adjacency matrix of a new undirected network,<sup>3</sup> and for this reason the method is considered to perform a graph transformation. Furthermore, the authors prove that in the produced undirected network, information about edge directionality is effectively incorporated as weights on the edges (entries of the matrix  $\mathbf{W}$ ). Moreover, a new definition of modularity is presented according to this approach, which is considered as a generalization of the one defined on undirected networks (e.g., see Section 2). The method is able to identify pattern-based clusters and more precisely, clusters that represent patterns of movement among the nodes of the network (flow-based clusters, Fig. 3(c)). The authors stress out that their method has broad applicability, since it can be used for several types of well-known directed networks (e.g., social and biological networks), as well as for networks where the edges represent patterns of movement among nodes that share common properties (e.g., the web graph, citation networks).

Later, the same authors presented a more extended approach [64], where edge directionality is extracted using a PageRank random walk (e.g., Ref. [35]), and introduced via weights on the edges of the transformed undirected network. The approach is more general regarding the types of cluster that are identified and introduces some interesting features. In contrast to the previous method which was based on the assumption that edges in the network capture only similarity between nodes, here the information about edges' direction is utilized in order to decide whether an edge lies inside a community (i.e., intra-community edge, connects two nodes that belong on the same community), or between communities (i.e., inter-community edge). Hence, the edges of the network are distinguished between inter-community and intra-community edges, very close to approaches presented for undirected networks. In other words, the information about the directionality of the edges, and thus the weights on the network, operate as an indicator of how likely the associated edges will belong on the same community; while the topological structure of the network is modified, the connectivity among nodes is preserved and the underlying community structure becomes more clear compared to the original network.

As we mentioned earlier, the method rely on the usage of random walks for directed networks in order to determine the structure of the network and to extract weights from edge directionality. The basic idea is the following: assume two nodes

<sup>3</sup> This is similar to the definition of Laplacian for undirected networks  $\mathbf{L}_U = \mathbf{D}_U - \mathbf{A}_U$ , where  $\mathbf{D}_U$  is the diagonal degree matrix and  $\mathbf{A}_U$  the adjacency matrix of the undirected network. See also Section 2.



**Fig. 8.** Example of transformation to bipartite graph. Each node of the directed network (a) is treated as a hub/authority or both, according to its out-degree/in-degree.

$A$  and  $B$  connected with an edge, and respective random walks starting from these two nodes. If both  $A$  and  $B$  are visited mutually during these random walks then the edge among those nodes is more likely to be an intra-community edge.

That is, according to the random walk, nodes that belong to the same community could interact more often among each other, and thus intra-community edges will receive higher weights than inter-community edges. The authors define the so-called *nodes' behavior vector*, where each entry represents the expected frequency with which the specific node will be visited by the random walk in  $t$  steps.<sup>4</sup> Then, the similarity between two such vectors (i.e., how similar are the trajectories of the random walks starting from these connected nodes) will be an indicator if these nodes belong on the same community. The authors suggest to apply two well-known similarity measures, namely the exponential and the cosine similarity. Having extracted the edge weights, the network can be treated as undirected and thus algorithms designed for undirected networks can be applied (the authors choose Newman's modularity optimization algorithm [40]). Finally, the proposed framework can identify flow-based clusters independently of the chosen clustering algorithm.

#### 4.2.2. Transformation to bipartite network

A somewhat different transformation approach than the ones presented earlier, assumes that the directed network is transformed into a bipartite undirected one and then community detection algorithms are applied on the latter. As we described in Section 2, bipartite networks form a special class of networks with interesting properties. Treating a directed network as bipartite is not something new, but it has been used in the past for other tasks in network analysis (e.g., Ref. [65]).

In the context of community detection for directed networks, the authors of Refs. [66,57] utilize a transformation scheme where a bipartite graph  $G_B = (V_h, V_a, E_b)$  is constructed from the original directed network  $G = (V, E)$ , according to the following process:

- $V_h = \{i_h | i \in V \text{ and } k_i^{\text{out}} > 0\}$
- $V_a = \{i_a | i \in V \text{ and } k_i^{\text{in}} > 0\}$
- Each directed edge  $(i, j) \in E$  between two nodes of the directed network  $G$ , will be represented by an edge  $(i_h, j_a) \in E_b$  between nodes  $i_h$  and  $j_a$  of the produced bipartite network  $G_B$ .

This implies that in the general case, the nodes of the directed network are doubled and each one is represented by a node at each of the two partitions. However, since some nodes may not have outgoing or incoming links (and thus they will be isolated in the resulting bipartite network), every node is placed in the two sets  $V_h, V_a$  according to its out- and in-degree respectively. Fig. 8 shows a construction of the bipartite network for a given directed one.

The above representation scheme is inspired by Kleinberg's *hub and authority* web model [62], where the web pages are distinguished in two sets: *authoritative pages* and *hub pages*. The first category includes web pages relevant to a specific topic, while the second one web pages that point to authorities of a relevant topic. Moreover, a web page can simultaneously belong to both sets.

In Ref. [66], the authors construct a bipartite network from the original directed one (adding all nodes to both sets of the bipartite graph), trying to identify clusters of nodes with similar outgoing links as well as similar incoming links. They distinguish the two partitions of the graph into the *actor* partition and *team* partition ( $V_h$  and  $V_a$  in our description). The ultimate goal is to identify groups of actors that are closely connected to each other through co-participation in many teams. To this end, their approach is based on the idea of modularity optimization. More precisely, they define a modularity function for bipartite networks, modifying Newman's modularity measure [40], and then apply an optimization technique based on simulated annealing for detecting the underlying community structure.

In a similar spirit, the authors of Ref. [67] propose an approach for revealing the community structure of bipartite and directed networks. They rely on the network transformation scheme presented above and suggest that every unipartite

<sup>4</sup> As the authors state, the length of the random walk should not be chosen too large (i.e., no greater than  $\log n$ ), even if it is not very crucial for the method's performance.

or directed network can be transformed to a bipartite one, while the modularity is preserved.<sup>5</sup> Then, an adaptive genetic algorithm called MAGA is presented, which according to the authors is capable to effectively optimize the objective function for the community structure detection problem (the authors select to apply the bipartite modularity function).

A different approach that based on the construction of a bipartite network is the one presented in Ref. [57]. The authors describe a framework for semi-supervised learning on directed networks, which can also be applied for the task of graph clustering. The framework was introduced for the problem of node classification in directed networks, where some nodes in the graph bear labels (positive or negative) and the goal is to classify unlabeled nodes. However, in case of absence of labeled node instances, the framework can be used as a graph clustering tool for both directed and bipartite networks. The main idea behind the approach is the so-called *category similarity of co-linked nodes* in directed networks; the existence of nodes with common parents (sibling structures) and nodes with common children (co-parent structures) should be taken into consideration at the clustering task since they can operate as indicators regarding node similarity (the general idea is similar with the one presented by Satuluri and Parthasarathy in Ref. [54]). The construction of a bipartite network from the original directed one is also inspired by Kleinberg's hub and authority web model, where co-linked node structures are highlighted.

#### 4.3. Extending objective functions and methodologies to directed networks

In the previous section, we presented methods where the graph clustering and community detection problem is not treated on the original directed network, but on a new undirected network that is produced applying meaningful transformation methods. The main advantage of these approaches is that they can benefit from the large bulk of techniques for the undirected case of the problem. However, the basic question behind such approaches remains the same: to what extend the information about the directionality of the edges is retained? To this direction, several methodologies have been proposed trying to deal with the problem without changing the structure of the original network. That is, instead of transforming the directed network to undirected, a different approach would be to transform or extend existing methods making them capable to work with directed networks.

Usually, two things need to be specified for the problem of clustering and community detection in networks. The first one has to do with the quality assessment of the produced clustering results, while the other is more general and is related to the algorithmic framework that will be applied to extract the community structure (according to how a “good” clustering should look like). In fact, these two things compose the basic steps of each clustering and community detection algorithm: (i) an objective function that quantifies the quality of a cluster and (ii) an algorithmic technique for optimizing this function. Both these aspects—questions have been treated for the case of undirected networks (or generally, several solutions have been proposed). In other words, there exist several objective measures for quantifying the quality of a clustering result, as well as algorithmic frameworks that are trying to optimize those objective criteria in order to identify and extract the underlying clustering structure of undirected networks (e.g., see Refs. [11,19]). Thus, a natural question would be if these quality measures and general methodologies can be extended to the case of directed networks and how this could be done.

In this section we present approaches for detecting clusters and communities in directed networks that constitute extensions of the undirected case. Note that, this category contains the most well-studied approaches for the clustering problem in directed networks. First, we will discuss well-known objective criteria that have been extended to take into consideration the directionality of the edges (e.g., modularity, cut-based measures). Then, we describe more general algorithmic frameworks that were initially introduced for clustering undirected networks and how they can be extended to the directed case. Such methodological frameworks include spectral clustering approaches based on the Laplacian matrix, as well as PageRank based and random-walk based methods. We must note here that some of these approaches are not independent. For example, several modularity-based methods apply spectral clustering in order to identify the best clusters. Whenever necessary, we briefly review the problem for the undirected case, trying to make this survey paper as self-contained as possible (see Section 2 for more details about the background, as well as other survey papers that focus on undirected networks).

##### 4.3.1. Modularity for directed networks

One of the basic objective criteria about the quality of a particular division into clusters for a network, is the so-called *modularity* function. Modularity was initially introduced by Newman and Girvan [40] for the case of undirected networks, as a measure for assessing the strength of the partitions produced by an hierarchical clustering algorithm (an thus indicating which partition should be kept). The measure is based on the idea that networks with inherent community structure usually deviate from random graphs. That is, since random graphs are not expected to have community structure, measuring the deviation between the concentration of edges in the original network from that someone expect in the case of random distributed edges, would be an indicator of the presence (or lack thereof) of community structure. Informally, the modularity score  $Q$  of each possible partition will be [40]:

$$Q = (\text{fraction of edges within communities}) - (\text{expected fraction of edges}). \quad (8)$$

<sup>5</sup> Some comments on the performance of the method have been proposed from other researchers [68].



Larger positive values of modularity indicate better community structure, since there are more edges within communities than one would expect if edges were placed in random (the maximum value of modularity can be 1). The expected fraction of edges among a group of nodes is usually based on the chosen configuration model, i.e., a random graph with the same degree sequence of the original network. In this model, the probability of an edge between two nodes  $i, j$  with degree  $k_i$  and  $k_j$  is  $k_i k_j / 2m$ , where  $m = \frac{1}{2} \sum_{i \in V} k_i$  is the total number of (undirected) edges in the network. Then, the modularity for undirected networks can be expressed as

$$Q_u = \frac{1}{2m} \sum_{i,j} \left[ A_{ij} - \frac{k_i k_j}{2m} \right] \delta(c_i, c_j), \quad (9)$$

where  $A_{ij}$  is the entry of the adjacency matrix which represents the existence or not of edge between nodes  $i$  and  $j$ ,  $\delta(c_i, c_j) = 1$  if  $c_i = c_j$  (i.e., if nodes  $i, j$  belong on the same community) and 0 otherwise.

Generally, modularity can be used both as quality measure for a specific network partition, as well as the basic ingredient of a framework for extracting the community structure. The latter procedure, usually called modularity optimization, is one of the dominant approaches for extracting the community structure in undirected networks (e.g., Ref. [41]).

In the case of directed networks, several extensions have been proposed for the measure of modularity. Arenas et al. [58] proposed a generalization for directed networks, where their ultimate goal was to reduce the size of the initial network (directed or undirected), while preserving the modularity value (this is a very crucial point since optimizing the modularity is a hard task). Their extension is based on the observation that the existence of a directed edge  $(i, j)$  between nodes  $i$  and  $j$ , depends on the out-degree and in-degree of nodes  $i$  and  $j$  respectively. Let us consider that node  $i$  has high out-degree but low in-degree, while node  $j$  has high in-degree and low out-degree. Then, it is more probable to observe the directed edge  $(i, j)$  from node  $i$  to node  $j$ , instead of observing edge  $(j, i)$ . Putting these insights together, the configuration model can be extended to the directed case, where an edge  $(i, j)$  from node  $i$  to node  $j$  will exist with probability  $k_i^{\text{out}} k_j^{\text{in}} / m$ . Then, the modularity function for directed networks can be expressed as

$$Q_d = \frac{1}{m} \sum_{i,j} \left[ A_{ij} - \frac{k_i^{\text{out}} k_j^{\text{in}}}{m} \right] \delta(c_i, c_j), \quad (10)$$

where the notation is similar to the one of Eq. (9). Also, observe that there is no factor of 2 in the denominator (the sum of out-degrees (similarly in-degrees) is equal to  $m$ ). Moreover, Arenas et al. [58] gave the relationship between directed and undirected modularity:

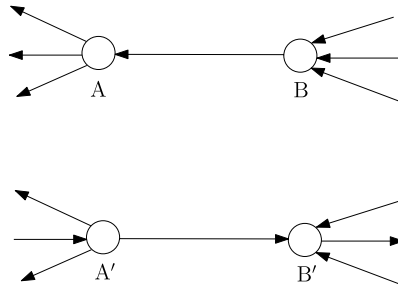
$$Q_d = Q_u + \frac{1}{4m^2} \sum_{i,j} (k_i^{\text{out}} - k_i^{\text{in}})(k_j^{\text{out}} - k_j^{\text{in}}) \delta(c_i, c_j). \quad (11)$$

Leicht and Newman [50] were based on the above definition of modularity to propose an algorithm for detecting communities in directed networks. Their approach constitutes a generalization of the modularity optimization method, presented by Newman and Girvan in Ref. [40], where modularity can be expressed in terms of the spectrum (eigenvalues and eigenvectors) of a special matrix called modularity matrix. More precisely, let us suppose that our goal is to assign the nodes of the network into two communities, namely  $\mathcal{A}$  and  $\mathcal{B}$ . Let  $s_i, \forall i \in V$  be an indicator variable taking value  $+1$  if vertex  $i$  is assigned to community  $\mathcal{A}$  and  $-1$  if is assigned to community  $\mathcal{B}$  and  $\mathbf{s}$  be the vector whose elements are the  $s_i$  values. Then, modularity can be written as

$$\begin{aligned} Q_d &= \frac{1}{m} \sum_{i,j} \left[ A_{ij} - \frac{k_i^{\text{out}} k_j^{\text{in}}}{m} \right] \delta(c_i, c_j) \\ &= \frac{1}{2m} \sum_{i,j} \left[ A_{ij} - \frac{k_i^{\text{out}} k_j^{\text{in}}}{m} \right] (s_i s_j + 1) \\ &= \frac{1}{2m} \sum_{i,j} B_{ij} s_i s_j \\ &= \frac{1}{2m} \mathbf{s}^T \mathbf{B} \mathbf{s}, \end{aligned} \quad (12)$$

where  $B_{ij} = A_{ij} - \frac{k_i^{\text{out}} k_j^{\text{in}}}{m}$  is the modularity matrix. In the general case matrix  $\mathbf{B}$  is not symmetric and thus we are not able to apply a spectral approach. However, transposing Eq. (12),  $Q_d$  can be expressed as  $Q_d = (2m)^{-1} \mathbf{s}^T \mathbf{B}^T \mathbf{s}$ . Finally, taking the average of this quantity with the one in Eq. (12) gives

$$Q_d = \frac{1}{4m} \mathbf{s}^T (\mathbf{B} + \mathbf{B}^T) \mathbf{s}. \quad (13)$$



**Fig. 9.** The modularity function introduced in Ref. [58] does not distinguish the directionality of the edges. Nodes  $A$  and  $A'$  as well as  $B$  and  $B'$  have the same in- and out- degree respectively. However, in the top figure there is a precise directed flow, while in the bottom no. Modularity cannot distinguish these different situations (Kim et al. [55]).

Source: Figure redesigned from Ref. [55].

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Matrix  $\mathbf{B} + \mathbf{B}^T$  is now symmetric. Thus, applying well-known approaches in optimization theory, a simple clustering algorithm can be derived from the spectrum of this matrix: compute the eigenvector that corresponds to the largest positive eigenvalue of the matrix  $\mathbf{B} + \mathbf{B}^T$  and assign the nodes to communities  $\mathcal{A}$  or  $\mathcal{B}$  according to the signs in the components of the eigenvector (generally, node  $i$  is associated with the  $i$ th component of the eigenvector).

Additionally, other optimization tools can be applied (e.g., see Section 2 and Ref. [11]). The above method can be extended to assign the nodes to more than two communities. This can be achieved by an iterative procedure which subdivides the produced communities until the modularity value is not increased. The algorithm has been tested on both synthetic and real datasets and the results show that, considering edge directionality in the modularity optimization process, meaningful communities can be identified (whereas ignoring the direction of the edges this cannot be achieved).

However, Kim et al. [55] observed that the directed version of modularity in Eq. (10) exhibits two limitations:

- (i) It cannot properly distinguish the directionality of the edges.
- (ii) It cannot be used to detect pattern-based clusters representing patterns of movement among nodes.

Fig. 9 presents an example where the directed modularity as introduced in Ref. [58] and used in the algorithm of Ref. [50], is not able to distinguish the two different cases. According to the modularity definition, nodes  $A$  and  $B$  are more likely to belong in the same community than nodes  $A'$  and  $B'$ , since the edge from  $B$  to  $A$  is more informative than the one from  $A'$  to  $B'$  (because of the fact that node  $B$  has small out-degree and node  $A$  small in-degree; thus the edge from  $B$  to  $A$  should contribute more to the modularity since it is a statistically surprising configuration). However, both edges have the same contribution to the directed modularity.

Based on the above observations, in Ref. [55] the authors proposed a somewhat different formulation of modularity for directed networks. Their approach, called LinkRank, is related to random walks and more specifically to Google's PageRank algorithm [69,35]. More precisely, LinkRank indicates the importance of links (edges) in the network (instead of nodes) as the probability that a random surfer will follow this link in the stationary state (similar to the definition of PageRank but now for the edges). That is, the LinkRank value of a particular edge  $(i, j)$  can be defined as

$$L_{ij} = \pi_i G_{ij}, \quad (14)$$

where  $\pi_i$  is the  $i$ th element of PageRank vector and  $G_{ij}$  is the element of Google matrix  $\mathbf{G}^6$  [69]. Then, a generalized version of modularity can be defined using random walk concepts as follows:

$$Q_{\text{linkrank}} = (\text{fraction of time spent by random surfer while walking within communities}) - (\text{expected value of this fraction}). \quad (15)$$

According to this modularity definition (which holds for both directed and undirected networks), a community is not just a group of nodes with more than expected number of edges, but a group of nodes where a random surfer is more likely to stay. Therefore, the directed modularity can be expressed as

$$Q_{\text{linkrank}} = \sum_{i,j} [L_{ij} - \pi_i \pi_j] \delta(c_i, c_j), \quad (16)$$

where  $\pi_i \pi_j = E(L_{ij})$  is the expected probability (in the configuration model) that a random surfer is moving from node  $i$  to  $j$  (and thus the expected value  $E(L_{ij})$  of  $L_{ij}$ ). Furthermore, the authors show that the proposed modularity measure  $Q_{\text{linkrank}}$  is

<sup>6</sup> Similar to the transition matrix  $\mathbf{P}$  but guaranteeing the existence of a stationary vector [69].

consistent with the original modularity  $Q_u$  of Eq. (9) for undirected networks. In other words, for undirected networks, the proposed definition of a community as a group of nodes where a random surfer is more likely to be trapped in is consistent with the traditional one, where a community represents a group of, more than expected, densely connected nodes. One other important feature is that the proposed LinkRank-based modularity function can be optimized using already existing methods [11], leading to a community discovery algorithm for directed networks. The authors claim that their method is able to detect mainly communities in directed networks where edges can be considered to represent citation/reference relationships (e.g., pattern-based clusters).

The same definition of modularity for directed networks was also presented in Ref. [56] (the method was also described in Section 4.2.1 since the original directed network is transformed into an undirected one). The method applies PageRank random walk to define the Laplacian matrix for the directed network, which at the end can be considered as a network embedding. Additionally, the authors provide an alternative definition of communities as nodes sharing common properties; nodes of the same group are more similar to each other compared to nodes outside the group. This can be also considered as a high level clustering definition, and is in agreement with the one we presented in Section 3.

In Refs. [70,71], Chang et al. present an alternative formulation of modularity (compared to  $Q_d$  of Eq. (10)), that relies on a different configuration model. As we described earlier, the configuration model used in  $Q_d$  [58,50] assumes that the existence of a directed edge from node  $i$  to node  $j$  is proportional to  $k_i^{\text{out}} k_j^{\text{in}} / m$ . The authors present a different configuration model that rely on the idea of conditional expected network (a similar approach has been presented for undirected networks [72]). That is, the configuration model can be formed by conditioning on the degrees (both in- and out-) of nodes in the original network as

$$E(A_{ij} | k_1^{\text{in}}, k_2^{\text{in}}, \dots, k_n^{\text{in}}, k_1^{\text{out}}, k_2^{\text{out}}, \dots, k_n^{\text{out}}) = E(A_{ij} | \mathbf{k}^{\text{in}}, \mathbf{k}^{\text{out}}). \quad (17)$$

The solution of the above conditional expected model suggested by the authors is considered for the case where the edges are distributed according to a Gaussian distribution and the final configuration model is the directed Gaussian random network (DGRN). A benefit of this model stands from the point that one can introduce prior information to the model in the form of the mean and covariance of the Gaussian distribution. Then, measuring the deviation from the configuration model, the modularity can be expressed as

$$Q_{dM} = \frac{1}{m} \sum_{i,j} [A_{ij} - E(M_{ij} | \mathbf{k}^{\text{in}}, \mathbf{k}^{\text{out}})] \delta(c_i, c_j). \quad (18)$$

Furthermore, using spectral techniques similar to the ones of Ref. [8] (or generally other modularity maximization algorithms), the modularity can be optimized obtaining a clustering assignment.

### Modularity for overlapping communities

In the discussion until now, we have reviewed approaches for the clustering and community detection problem, where each node is assigned into just one community with no overlaps among communities. However, a different version of the problem is to allow nodes to be assigned in more than one communities, leading to the concept of *overlapping communities*. The intuition behind overlapping clustering is based on the fact that real complex networks usually are not divided into sharp sub-networks, but typically nodes may naturally belong to more than one communities. For instance, in a social relationship network, individuals usually belong to several different communities at the same time (family's community, friendship's community, profession's community, etc.). Thus, being able to identify the overlapping communities of directed networks, could offer fruitful insights about network structure.

To this direction, Nicosia et al. [73] extended the measure of modularity to the more general case of directed networks with overlapping communities. The main point of their approach is to extend the configuration model that is used in the definition of modularity [50], allowing nodes to belong to several communities at the same time. Typically, nodes belong to each community with a certain strength and each node  $i \in V$  is associated with a coefficient  $\alpha_{i,c}$  that indicates how strongly this node belongs to community  $c$  (i.e., each node  $i$  is associated with a vector  $[\alpha_{i,1}, \alpha_{i,2}, \dots, \alpha_{i,|c|}]^T$ , where  $|c|$  the total number of communities). Then, a similar coefficient can be defined for the participation of edges to communities; for each directed edge  $e = (i, j)$  the belonging factor to community  $c$  can be represented by a function of the corresponding coefficients of nodes  $i, j$ , i.e.,  $\beta_{e,c} = \mathcal{F}(\alpha_{i,c}, \alpha_{j,c})$ . Then, the  $\delta(c_i, c_j)$  function can be substituted by two different coefficients  $r_{ijc}$  and  $s_{ijc}$ , regarding the contribution of edge  $(i, j)$  to the modularity of the network and the configuration model respectively. Finally, the modularity can be expressed as

$$Q_{ov} = \frac{1}{m} \sum_c \sum_{i,j} \left[ r_{ijc} A_{ij} - s_{ijc} \frac{k_i^{\text{out}} k_j^{\text{in}}}{m} \right]. \quad (19)$$

One can observe that if there is no overlap between communities, then  $r_{ijc} = s_{ijc} = \delta(c_i, c_j)$ , where the edge  $(i, j)$  contributes to modularity only if  $c_i = c_j$ . The value  $r_{ijc}$  can be thought of as the contribution of edge  $e = (i, j)$  to the modularity of community  $c$  and according to the above discussion,  $r_{ijc} = \beta_{e,c} = \mathcal{F}(\alpha_{i,c}, \alpha_{j,c})$ . For the factor  $s_{ijc}$  that is related to the configuration model, assuming that the belonging of a node to a community is independent from the belonging of every other node on the same community (i.e., the probability that a node  $i$  belongs to community  $c$  with strength  $\alpha_{i,c}$  is not

related to the probability that any other node  $j$  belongs to the same community with strength  $\alpha_{j,c}$ , the modularity can be defined as

$$Q_{ov} = \frac{1}{m} \sum_{\forall c} \sum_{i,j} \left[ r_{ijc} A_{ij} - s_{ijc} \frac{\beta_{e,c}^{out} k_i^{out} \beta_{e,c}^{in} k_j^{in}}{m} \right], \quad (20)$$

where

$$\beta_{e,c}^{out} = \frac{\sum_{j \in V} \mathcal{F}(\alpha_{i,c}, \alpha_j, c)}{|V|} \quad \text{and} \quad \beta_{e,c}^{in} = \frac{\sum_{j \in V} \mathcal{F}(\alpha_{i,c}, \alpha_j, c)}{|V|} \quad (21)$$

are the expected belonging coefficients of any edge  $e = (i, j)$ , where node  $i$  belong to community  $c$  (i.e., the average membership for all edges). One more thing needs to be specified for defining the modularity measure for directed networks with overlapping communities and it concerns the selection of function  $\mathcal{F}(\alpha_{i,c}, \alpha_j, c)$  which specifies the belonging of an edge  $(i, j)$  in a community  $c$  according to the belonging coefficients of the end nodes  $i, j$ . The authors suggest that the selection of the  $\mathcal{F}(\cdot)$  function should lead to a valid modularity measure: (i)  $Q_{ov}$  should equals to zero when no community structure can be identified and all nodes belong to the same community and (ii) higher value of  $Q_{ov}$  indicates better community structure. Every potential function that preserves these properties can be applied to modularity. Finally, the authors present a genetic algorithm for optimizing the proposed modularity criterion, and therefore it can be used to identify the underlying overlapping community structure in directed networks.

#### Local definition of modularity

The definitions for the directed version of modularity that we have presented so far, assume that in the configuration model (the random graph model competitor), each node could be equally connected to any other node in the network. That is, the probability of an edge between every pair of nodes is the same, independent of the relative position of the nodes in the graph. In Ref. [74], Muff et al. propose a local definition of modularity for directed networks, where the expected number of edges within each community  $c$  is computed with respect to the subgraph consisting of the community  $c$  and its neighbor communities (and not based on the full network). That is, a local function of modularity can be expressed as

$$Q_{local} = \sum_{\forall c \in C} \left[ \frac{L_c}{L_{cN}} - \frac{k_c^{out} k_c^{in}}{L_{cN}^2} \right], \quad (22)$$

where  $L_c$  is the number of edges within community  $c$ ,  $L_{cN}$  the number of edges contained in  $c$ 's neighbor communities and  $k_c^{out}$  ( $k_c^{in}$ ) the total external (internal) degree of community  $c$ . The authors provide experimental results where the maximization of  $Q_{local}$  provides more cohesive partitions in a school network dataset (interactions among students and their classmates) as well as in the metabolic network of *E. coli*.

#### Discussion

As discussed in Section 2, the modularity function suffers from the so-called *resolution limit* [49], i.e., modularity optimization may fail to identify communities smaller than a specific size that depends on the scale of the network. This limitation was initially found in the undirected version of modularity ( $Q_u$  in Eq. (9)), but a similar behavior is expected for the extension in directed networks (as we mentioned earlier, there is a close connection between  $Q_u$  and  $Q_d$  [58]). Thus, the produced partition that maximizes modularity may correspond either to single communities or to a merging of smaller weakly connected communities. In the literature, some possible meta-algorithmic approaches have been proposed, that can help to overcome the resolution limit [11].

#### 4.3.2. Spectral clustering and cut-based measures for directed networks

In this section, we will review methodologies for the clustering problem in directed networks that are based on the concept of spectral clustering and graph cuts, and we will present the close relationship between them; these methods mainly constitute extensions of popular clustering approaches from the undirected case.

The algorithmic framework of spectral clustering was initially considered for the case of undirected networks, and includes methods that partition the nodes of a graph into clusters using information related to the spectrum of a matrix representation of the dataset (e.g., Laplacian or adjacency matrix). Spectral methods can be applied not only in networks (graph structures), but generally in every set of  $N$  objects where a pairwise similarity function between them can be defined. For a nice tutorial about spectral graph clustering, one can refer to the survey paper of von-Luxburg [14]. Here we will present extensions to directed networks and more precise, we will examine the generalization of the Laplacian matrix for directed graphs.

Furthermore, spectral clustering methods can also be applied in a slightly different way for solving the graph clustering problem. This can be achieved through their close connection with the cut-based graph clustering method. Broadly speaking, in the graph clustering problem the goal is to partition the nodes of a network, in such a way that the edges between different groups should have low weight (or in the case of unweighted networks, the number of edges should be small), while the

edges within a group should have high weight (note that the total weight of every cluster is considered aggregating the weights of edges). In other words, there are two criteria of interest when quantifying how good a community or a cluster is. The first one considers the number of edges between the nodes of the cluster, while the second the number of edges between nodes of the candidate community with the rest of network. As noted in Section 2, the objective functions for the clustering problem can be formed according to one of these criteria (single-criterion scores) or based on a combination of them (multi-criterion scores) [39].

However, the optimization of these objective cut-based criteria typically lead to computational difficult problems, but relaxed versions of them can be turned into spectral clustering problems. The optimization measures can be expressed in a matrix form and then the spectrum (eigenvectors) of this matrix can be used to obtain the final clusters. We remind here that something similar was presented in Section 4.3.1 for the optimization of modularity. In that case, the modularity was expressed in a matrix form and applying spectral techniques the partition that maximizes modularity was detected. Thus, it is clear that spectral methods have a dual use: either as clustering framework itself or as an optimization framework for objective functions. For the latter case, first we will present how cut-based measures can be extended to directed networks and then how spectral methods can be applied on them as an optimization process. In the next section, we will discuss about the connections between cuts, spectral clustering and random walks on graphs.

#### Laplacian matrix for directed networks

The Laplacian matrix of an undirected graph [31] is one of the main tools for spectral clustering. As we discussed in Section 2, the eigenvector that corresponds to the second smallest non-zero eigenvalue of the Laplacian matrix (the so-called Fiedler vector) can be used to obtain a bi-partition of the nodes of the graph into two sets  $S, \bar{S} = V - S$  with relatively small number of edges connecting the two sets (this can be achieved through the well-known Cheeger inequality). That is, the eigenvectors of the Laplacian matrix provide a solution to the *normalized cut* objective function, which captures the clustering notion of a subset  $S$  as (see also Ref. [38] by Shi and Malik):

$$\text{NCut}(S, \bar{S}) = \text{Cut}(S, \bar{S}) \left( \frac{1}{\text{Vol}(S)} + \frac{1}{\text{Vol}(\bar{S})} \right), \quad (23)$$

where  $\text{Cut}(S, \bar{S}) = |\{(i, j) : i \in S, j \in \bar{S}\}| = \sum_{i \in S, j \in \bar{S}} A_{ij}$  and  $\text{Vol}(S) = \sum_{j \in S, t \in V} A_{jt}$  is the total number of edges starting from nodes in  $S$ . Then, the optimal bi-partition of the graph is the one that minimizes the normalized cut value and this can be approximated by the spectrum of the Laplacian matrix.

In the case of directed graphs, how the above property is generalized? The answer was initially provided by Chung [17], who proposed a version of the Laplacian matrix for directed networks, based on a random walk process. That is, for a directed network  $G$  the Laplacian matrix can be defined as

$$\mathbf{L}_d = \mathbf{I} - \frac{\boldsymbol{\Pi}^{1/2} \mathbf{P} \boldsymbol{\Pi}^{-1/2} + \boldsymbol{\Pi}^{-1/2} \mathbf{P}^T \boldsymbol{\Pi}^{1/2}}{2}, \quad (24)$$

where  $\mathbf{P}$  is the transition matrix, i.e.,  $P_{ij} = \frac{A_{ij}}{k_i^{\text{out}}}$  and  $\boldsymbol{\Pi} = \text{diag}(\pi_1, \dots, \pi_n)$  the diagonal matrix with the probability of finding the random walk on each vertex (the stationary distribution of the random walk). (One can observe that the matrix is the same with the one used by Ref. [56] in Eq. (7)). Moreover, the most important point is that the Laplacian matrix of Eq. (24) satisfies the so-called Cheeger inequality, making it a useful tool for the graph clustering problem. In other words, the eigenvector of the second smallest non-zero eigenvalue of  $\mathbf{L}_d$  can be used to approximate a good cut in the network. Another version of the Laplacian matrix for directed networks (called Diaplacian) with similar interesting properties, was recently presented by Li and Zhang in Refs. [32,33].

Based on Chung's extension of the Laplacian matrix for directed networks, Gleich [75] proposed an hierarchical spectral graph clustering algorithm for directed networks. The idea utilizes Cheeger inequality that holds for the new directed Laplacian matrix and by recursively using the eigenvector  $\mathbf{u}_1$  that corresponds to the second smallest non-zero eigenvalue  $\lambda_1$ , a partition of the graph into two clusters can be achieved. The author suggests that this recursive process can terminate when the resulting subgraph contains less than  $p$  nodes. Moreover, a possible extension of the algorithm to higher eigenvectors is discussed, where each higher eigenvector (other than  $\mathbf{u}_1$ ) offers the next best solution for the normalized cut. That is, the spectrum of the directed Laplacian matrix ( $k$  smallest eigenpairs) can be used to partition the network into  $c$  clusters.

A similar solution to the problem was proposed by Zhou et al. [61], who considered a normalized analogous of the directed Laplacian matrix. More precisely, the authors define the matrix

$$\boldsymbol{\Theta} = (\boldsymbol{\Pi}^{1/2} \mathbf{P} \boldsymbol{\Pi}^{-1/2} + \boldsymbol{\Pi}^{-1/2} \mathbf{P}^T \boldsymbol{\Pi}^{1/2})/2, \quad (25)$$

where  $\mathbf{L}_d = \mathbf{I} - \boldsymbol{\Theta}$ . According to this relation between  $\mathbf{L}_d$  and  $\boldsymbol{\Theta}$ , the best normalized cut will correspond to the eigenvector of the second largest eigenvalue of  $\boldsymbol{\Theta}$  (instead of second smallest in the case of  $\mathbf{L}_d$ ). Algorithm 1 describes the pseudocode of the clustering algorithm for directed networks based on the above discussion, where the graph is partitioned into two parts (the algorithm is similar to the one presented by Gleich in Ref. [75]).

The above algorithm can be extended in the case of a  $k$ -partition (instead of a bi-partition), considering the eigenvectors that correspond to the  $k$  largest eigenvalues of  $\boldsymbol{\Theta}$ . Furthermore, in the case of labeled data (where each node is associated



**Algorithm 1** Directed Spectral ClusteringINPUT: Directed graph  $G = (V, E)$ OUTPUT: A partition of the vertex set  $V$  into two parts, minimizing the normalized cut

- 1: Define a random walk over  $G$  with transition matrix  $\mathbf{P}$ .
- 2: Form the matrix  $\mathbf{\Theta} = (\mathbf{\Pi}^{1/2}\mathbf{P}\mathbf{\Pi}^{-1/2} + \mathbf{\Pi}^{-1/2}\mathbf{P}^T\mathbf{\Pi}^{1/2})/2$ , where  $\mathbf{\Pi}$  is the diagonal matrix with elements being the stationary distribution of the random walk.
- 3: Compute the eigenvector  $\mathbf{u}_2$  of  $\mathbf{\Theta}$  that corresponds to the second largest eigenvalue; then partition the vertex set  $V$  into two parts  $S = \{i \in V | \mathbf{u}_2(i) \geq 0\}$  and  $S' = \{i \in V | \mathbf{u}_2(i) < 0\}$ .

with a label), the above methodology can be used as a general learning (classification) framework for directed networks. Later, the framework was extended to the case of graphs with multiple views, where data is associated with multiple representations [76]. For example, in the case of the web graph, each web page can be represented either as a node in a directed network based on the hyperlink structure, or using the vector-space model based on occurrences of words in a web page. These two different views can be combined as a directed hyperlink network, weighted according to the similarity of the web pages. In the general case, each different view can be represented as a directed network with the same set of nodes  $V$  and the idea is to combine these different views to improve the accuracy of the learning framework (e.g., the graph clustering task).

*Cut-based measures for directed networks*

A basic point of the Laplacian-based spectral clustering algorithm that we presented above, is that it provides a solution to the normalized cut problem. The objective criterion that is optimized while using the eigenvectors of the Laplacian matrix (of a directed or undirected network), is a generalized version of the normalized cut. Additionally, other possible cut-based objective criteria can also be applied to the clustering problem in directed networks, as the one of weighted cuts proposed by Meilă and Pentney [59]. More precisely, the authors introduced the *generalized weighted cut* criterion, defined as follows

$$\text{WCut}(S, \bar{S}) = \frac{\sum_{i \in S, j \in \bar{S}} T'_i A_{ij}}{\sum_{i \in S} T_i} + \frac{\sum_{j \in \bar{S}, i \in S} T'_j A_{ji}}{\sum_{j \in \bar{S}} T_j}. \quad (26)$$

One can observe that this criterion is similar to the one of normalized cut (Eq. (23)), but it is parametrized by the vectors  $T$  and  $T'$ . That is, the objective is to form node clusters of balanced size, where clusters' size is parametrized by vector  $T$ , while vector  $T'$  plays the role of a normalization factor for the adjacency matrix  $\mathbf{A}$ . An important point is that different normalized cut-based measures can be recovered from the definition of WCut, by properly setting the parameter vectors  $T$  and  $T'$ . This point makes the new criterion more flexible. The authors show that the optimization of the WCut function can be relaxed on an analogous symmetric problem, where many existing spectral clustering algorithms and theoretical results can be applied for extracting the final clusters. The experimental results show that the symmetrized version of the spectral clustering problem produced by the weighted cut objective function, gives better results compared to the cases where the matrix is symmetrized using simple linear algebraic transformations (e.g., some of those presented in Section 4.2.1).

In the context of image processing and analysis, the authors of Ref. [77] present an approach for clustering directed networks, generalizing the normalized cuts criterion. At a first point, a new representation scheme is proposed, in which all possible pairwise relationships are characterized according to two types of node correlations, namely *attraction* and *repulsion*. According to these relationships, the general compatibility between two pixels in the image can be captured by two different directed networks that correspond to each of these two relationships. The general idea behind the approach is that at the clustering process, the attraction of nodes that belong on the same group should be as large as possible, while the repulsion between two different groups should be minimized. Then, information about these two graphs is introduced in a “dual” clustering criterion that extends the notion of normalized cuts. Finally, the optimization of the produced objective functions leads to an eigendecomposition problem of a Hermitian matrix, where the imaginary part encodes directed relationships, while the real part encodes undirected relationships with positive numbers for attraction and negative numbers for repulsion.

*4.3.3. PageRank and random walk based methods*

The PageRank and generally random walks over graphs are closely related to spectral clustering. That is, cut-based measures in networks (e.g., normalized cuts) and their optimization process, can be expressed in terms of random walks [78]. Broadly speaking, the minimization of the number of edges that crossing a cut in a network can be described as a similar process where the random surfer is forced to stay more time within a cluster. In other words, the normalized cut objective criterion presented in Eq. (23), corresponds to the probability of the random walk transitioning from the vertex set  $S$  to set

$\bar{S}$  in one step if it is currently in  $S$  and the random walk is started in the stationary distribution (or vice-versa):

$$\text{NCut}(S, \bar{S}) = \frac{\Pr(S \rightarrow \bar{S})}{\Pr(S)} + \frac{\Pr(\bar{S} \rightarrow S)}{\Pr(\bar{S})}. \quad (27)$$

That is, if  $\pi$  represents the stationary distribution of the random walk, then the probability  $\Pr(S)$  with which the random surfer can be found in a node in  $S$  can be defined as  $\Pr(S) = \sum_{i \in S} \pi_i$  (similarly for  $\Pr(\bar{S})$  and also  $\Pr(S) + \Pr(\bar{S}) = 1$ ). Then, the probability that the random walk will move from  $S$  to  $\bar{S}$  can be defined as  $\Pr(S \rightarrow \bar{S}) = \sum_{i \in S, j \in \bar{S}} \pi_i P_{ij}$ , where  $\mathbf{P} = [P_{ij}]_{i,j \in V}$  is the transition matrix.

Equation (27) considers the general case of graphs with the existence of directed edges and thus can be naturally applied in directed networks (in the case of undirected networks  $\Pr(S \rightarrow \bar{S}) = \Pr(\bar{S} \rightarrow S)$ , since the probability of transition from  $S$  to  $\bar{S}$  is equal to the one from  $\bar{S}$  to  $S$ ). As we described in Section 4.3.2, this criterion can be approximated by the eigenvalues of the Laplacian matrix for directed networks [61].

It also holds for undirected networks that relying only on the first top  $k$  eigenvectors of the transition matrix  $\mathbf{P}$  which is related to the random walk, one is able to identify the underlying clusters [79]. A similar result was presented for directed networks, which states that a clustering can be achieved by looking for piecewise constant eigenvectors in the transition matrix  $\mathbf{P}$  [80]. However, as noted by Capocci et al. [81], one can rely on the eigenvectors of matrix  $\mathbf{P}$ , if the network has a clear modular structure. However, in practice, this is something that occurs rarely; typically, real large networks have no clear community structure, and the eigenvector components do not show a clear step-wise form. To deal with this issue, Capocci et al. [81] presented an approach where the underlying community structure is revealed by correlations between the same components of different eigenvectors. That is, the eigenvector components that correspond to nodes of the same cluster, will show high correlation among each other. In the case of directed networks, the adjacency matrix of the network is replaced by matrix  $\mathbf{A}\mathbf{A}^T$  and a similar methodology is applied (therefore the method first transforms the directed network to undirected by a transformation approach which introduces edges between nodes with common neighbors).

In the context of community detection in the directed Web graph, Huang et al. [82] proposed to extend the random-walk based approach, using some variations of random walks that are able to identify latent Web communities. That is, instead of only satisfying a normalized cut criterion where two web pages (nodes) are assumed to be related if they are directly connected, the authors also consider the case of pattern-based clusters where co-citation and co-reference information is taken into consideration. In other words, the random walk should ensure that Web pages that share a common topic or interest should be grouped together, even if they are not directly connected (the case of pattern-based clusters that we described in Section 3.2). More precisely, their first approach involves two versions of the *PageRank random walk* (or teleporting random walk) [35], one following the forward hyperlinks while the other the backward ones. The first one can be considered as an authority-based ranking of nodes while the second as hub-based (e.g., see Ref. [62]). Moreover, PageRank guarantees the convergence to a stationary distribution through the adoption of a damping factor (in case of absence of in/out edges for a node). In their second approach, the authors consider a two-step random walk, in order to reveal latent communities that imposed by the existence of co-citation and co-reference edges. That is, starting from a node  $u$ , the random surfer first jumps one hop backward to a hub node  $h$  with probability  $P_{uh}^- = A_{hu}/k_u^{\text{in}}$ , and then she moves one step forward to a node  $v$  (adjacent to  $h$ ) with probability  $P_{hv}^+ = A_{hv}/k_h^{\text{out}}$ . Then, the two-step transition probability between authorities  $u, v$  is defined as

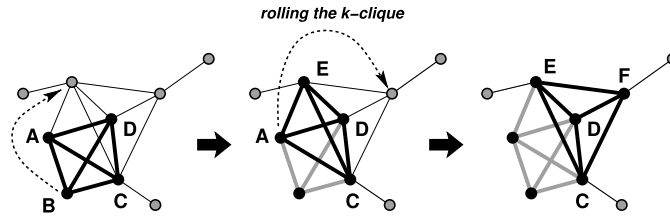
$$P_{uv}^A = \sum_h P_{uh}^- P_{hv}^+, \quad (28)$$

where nodes are treated as authorities. Similarly, forcing the random surfer to move firstly one step forward and then one step backward, the nodes are treated as hubs, and the transition probability matrix  $\mathbf{P}^H$  can be similarly defined. Moreover, since both these two-step random walks require that each node should have incoming and outgoing edges, again a teleporting probability (damping factor) is introduced. Finally, the above two types of random walks can be combined through a convex combination, in order to consider both co-citation and co-reference node similarity. In this case, the transition matrix can be expressed as  $\mathbf{P} = \beta \mathbf{P}^A + (1 - \beta) \mathbf{P}^H$ , where parameter  $\beta$  controls the co-citation and co-reference effects. Since the modified transition matrix  $\mathbf{P}$  has been defined, it can be applied to the Laplacian matrix of Eq. (25), and spectral methods can be used to extract the clusters.

A similar PageRank-based approach for clustering hypertext document collections that are represented by directed networks, was introduced in Ref. [83]. The proposed algorithm (called PRC) is composed by two parts. In a first step, a set of centroid nodes are selected (according to a node ranking criterion such as PageRank or Hits), and after that, the nodes are assigned to clusters using a Personalized PageRank method<sup>7</sup> (also called topic-specific or local PageRank) [84], combined with similar spectral optimization tools like those presented earlier.

In Ref. [85] the authors combined random walks with the concept of affinity propagation [86] and proposed a message passing algorithm for community detection in both directed and undirected networks. Affinity propagation is a mechanism

<sup>7</sup> This is a variant of the PageRank algorithm where a set of nodes is favored by the random walk. That is, the probability that the random surfer will jump to a node in a teleport step is not uniform for all nodes (as in the PageRank algorithm). In the extreme case, only one node is favored.



**Fig. 10.** Illustration of the Clique Percolation Method for undirected networks [88]. Initially, a template  $k$ -clique ( $k = 4$ ) is placed on nodes A–B–C–D. The template is gradually rolled to adjacent  $k$ -cliques and the final module consists of nodes A–B–C–D–E–F.

Source: The figure is courtesy of Palla et al. [88].

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that has been previously used in the task of clustering data points, where each group is associated with a representative point. Broadly speaking, the method of community detection via affinity propagation can be likened to an election process, in which nodes represent voters and the group leaders are the representative nodes. Through message passing along the edges of the network, the nodes are able to identify the community that they belong to; this is determined by its community leader, examining the similarity with their neighbors. The similarity between two nodes is computed using random walks and a variant of the transition matrix; each node is finally represented as a vector in  $\mathbb{R}^n$  and well-known similarity metrics are applied (e.g., cosine similarity).

A somewhat different version of the problem is the one of local graph partitioning, where instead of clustering the whole graph, the goal is to find a “good” local clustering structure near a specified seed node, by examining only a small portion of the input graph. As we will discuss later at this paper, this is a very interesting variant of the community detection problem. In Ref. [87], Andersen et al. propose a local clustering algorithm for directed networks (extending a similar method for undirected networks), combining information from both the Personalized PageRank score of a node  $v$  and the global one (i.e., the classical version of PageRank). That is, for a specific seed node, the authors compute the Personalized PageRank score with a single starting node (the seed node), as well as a global PageRank score with a uniform starting distribution over all nodes. Then, it is proved that taking the ratio of the entries in the Personalized PageRank and global PageRank vectors and sorting the nodes of the graph according to this ratio, one is able to identify a local set of nodes (cluster) with good clustering properties. The quality of the obtained cluster is determined by the measure of conductance (e.g., see Ref. [39]) which is generalized for directed networks.

#### 4.3.4. Other extensions

In this section we describe a few other diverse approaches for detecting communities in directed networks, that mainly extend concepts from the undirected case of the problem.

##### *Clique percolation method for overlapping community detection*

Palla et al. [88] presented a technique which extends the *clique percolation method* initially proposed for undirected networks. The goal of the method is to detect network modules (i.e., dense connected groups of nodes), following a local search approach based on edge density. Moreover, the produced modules may overlap with each other (i.e., a node may belong to more than one communities). In the case of undirected networks, the clique percolation method considers that the definition of modules is based on adjacent  $k$ -cliques. A  $k$ -clique is a complete subgraph with  $k$  nodes, while two  $k$ -cliques are adjacent if they share  $k - 1$  nodes. A module is defined to be the union of  $k$ -cliques that can be reached from each other traversing the edges of adjacent  $k$ -cliques. In other words, considering a  $k$ -clique as a template, the modules can be identified by rolling the template to an adjacent  $k$ -clique (retaining all but one node fixed) as shown in Fig. 10.

The method is extended in directed networks, defining the concept of directed  $k$ -cliques as complete subgraphs of size  $k$ , where the nodes can be ordered such that between any pair of nodes there is a directed edge from a higher order node to a lower one. The ordering is obtained according to the restricted out-degree of a node in the  $k$ -clique (the number of out-neighbors in the clique). Then, the directed  $k$ -clique modules are defined in a similar way as in the undirected case, by considering the union of adjacent directed  $k$ -cliques. The authors discuss that the proposed definition of  $k$ -cliques for directed networks is not unique, and other extensions can be considered as well.

##### *Local density clustering*

One other clustering method that aims to detect clusters based solely on local information, is the one presented by Schaeffer and Virtanen in Refs. [89,90] respectively. The basic idea of the approach is to extend the concept of cluster density to directed networks. (The problem is similar to the one presented earlier in Section 4.3.3 about local graph partitioning). More precisely, a local search method is applied in order to find a good cluster that contains a specified seed node (the approach can be naturally extended to several seed nodes). That is, the internal degree of a local cluster  $C \subseteq V$  is defined as  $\text{int-deg}(C) = |\{(u, v) \in E | u, v \in C\}|$  (i.e., the number of edges with both endpoints in  $C$ ), while the external degree is  $\text{ext-deg}(C) = |\{(u, v) \in E | u \in C, v \notin C\}|$  (i.e., the number of directed edges  $(u, v)$  that have only the start node  $u$  in  $C$ ). The density of the directed network  $G = (V, E)$  is defined as  $\delta = \frac{m}{n(n-1)}$ , where  $m = |E|$  and  $n = |V|$ . Similarly, the density of a

cluster  $C$  (also called local density) can be defined as  $\delta_\ell(C) = \frac{\text{int-deg}(C)}{|C|(|C|-1)}$  and the relative density as  $\delta_r(C) = \frac{\text{int-deg}(C)}{\text{int-deg}(C) + \text{ext-deg}(C)}$ . The authors combine the local and relative density and the final quality measure is selected to be the product of them:  $f(C) = \delta_\ell(C) \cdot \delta_r(C)$ . Having defined the clustering quality function, the problem of local clustering can be stated as follows: find a subgraph  $C$  with  $k$  nodes (i.e., the cluster) that contains a given node  $v \in V$ , maximizing  $f(C)$ . Since this is a computational difficult problem, the authors propose a local search approach starting from node  $v$  and gradually expanding the subgraph around  $v$ .

#### 4.4. Alternative approaches for community detection in directed networks

In this section we review “alternative” clustering approaches for directed networks that do not belong to one of the previous categories. While the approaches described so far either transform the original directed network to undirected or constitute well-known extensions from undirected to directed networks, here we will review algorithms that follow different and diverse methodological approaches. We classify them in three categories, according to the main methodology they follow, namely (a) information-theoretic, (b) mixture models and statistical inference, and (c) stochastic blockmodels. One additional category is devoted to approaches that mainly deal with variations of the clustering problem (e.g., community detection in dynamic directed networks). We note that even some of these approaches have been applied in the past on undirected networks, we decide to review them independently, trying to identify and demonstrate additional concepts that can be used for the problem. Moreover, some of them can be applied on both directed and undirected networks (i.e., independent from edge directionality), and we briefly discuss about this interesting feature. Although categories (b) and (c) both refer to approaches on probabilistic models, we decide to review them independently, since they are based on different statistical inference techniques.

##### 4.4.1. Information-theoretic based approaches

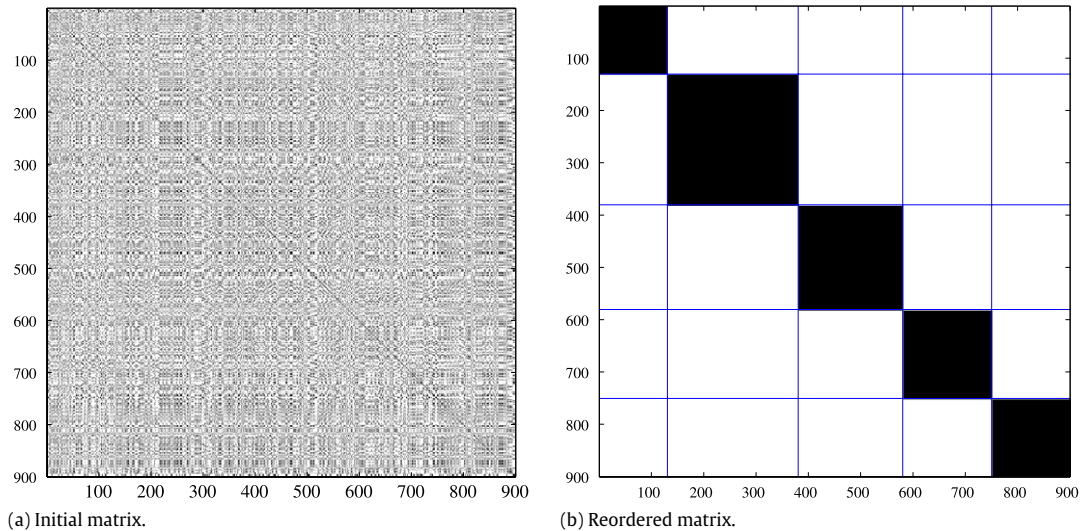
A prominent methodology for extracting the community structure of a network is the one that applies information-theoretic and compression principles. Generally, the existence of communities in networks represent structural patterns and regularities, that similar to more traditional data mining and analysis tasks, they can be used to effectively compress the network (data), e.g., Refs. [91,92]. Rosvall and Bergstrom [18] proposed a method (called Isomap) to identify communities in directed networks, by combining random walks and compression principles. That is, the modules of the network can be recognized based on how fast information flows on them. The authors apply the concept of random walks to describe the process of information flow in the network and the clusters can be extracted by compressing the description of the random walk. As we have already discussed, a community corresponds to a group of nodes in which the random surfer is more likely to be trapped in, visiting more time nodes of the group than other nodes outside of that. Thus, intuitively, a community would correspond to a group of nodes in which the random walk can be compressed better and the problem can be reformulated as a coding one: the goal is to select a partition  $M$  of the  $n$  nodes into  $c$  communities, minimizing the description length of the random walk.

At a first step, each node in the network is described by a unique codeword based on the visiting frequency of the random walk. Using Huffman coding, shorter codewords are assigned to more frequently visited nodes. At a second step, the random walk trajectory on the network can be described following a two-level description: unique names (codewords) are assigned to the clusters of the network (coarse-grained structure), while the codewords for the description of nodes inside a module are reused (fine-grained structure). Thus, reporting only the codewords that have been assigned to communities, a coarse-grained description of the network is achieved. The procedure is similar to the one used while designing a geographic map; unique names are assigned to cities (communities in our case), while names for the streets (nodes in our case) of a city can be reused. Then, the clustering problem can be expressed as finding the partition that yields the minimum description code length. If the network has a well-defined community structure, the above two-level description scheme will produce shorter code length: the random walk will jump between different communities infrequently and thus the description length will be shorter (since the codewords representing individual nodes are shorter). The minimization of the description length can be achieved combining greedy search and simulated annealing methods. Regarding the clustering results, the Isomap algorithm is able to identify pattern-based clusters and more specifically clusters of flow patterns induced by the edges of the network.

A somewhat different formulation of information theoretic principles in the community detection problem has been presented by Chakrabarti in Ref. [93] (even though the algorithm is tested on undirected networks, it seems that it can be applied in directed networks as well). The proposed algorithm (called AutoPart) can be considered as a co-clustering tool for binary matrices (the adjacency matrix in our case), where compression concepts are applied to identify the underlying clustering structure.<sup>8</sup> The goal of the algorithm is to group the nodes of the network into clusters in such a way that the adjacency matrix will be divided into rectangular, homogeneous blocks of high or low density, indicating that the certain node groups have more (or less) connections with other groups (e.g., Fig. 11). This can be achieved through a reordering procedure of the adjacency matrix, where the rows and columns of the matrix are rearranged to achieve this

<sup>8</sup> The term co-clustering refers to the task of simultaneously clustering the rows and columns of a matrix. As we will present later in this Section, the formulation of the co-clustering problem is similar to the blockmodeling approach.





**Fig. 11.** An example of the community detection algorithm through co-clustering: (a) The initial adjacency matrix. (b) The columns and rows of the matrix are reordered forming homogeneous blocks that can be used to better compress the matrix. At the end, these blocks correspond to co-clusters.  
Source: Figures redesigned from Ref. [93].

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structure. The quality of different possible clustering structures is evaluated in terms of the total compression cost  $T$ . That is, the best compression scheme should achieve a tradeoff between the number of produced blocks (i.e., clusters) and how homogeneous these blocks are. In the two extreme cases, one could select either only one block (the whole matrix) but not very homogeneous, or  $n^2$  perfectly homogeneous blocks of size 1 (each cell of the matrix). This tradeoff is achieved applying the Minimum Description Length principle (MDL) for model selection: the best clustering (model) is the one that minimizes the compression cost of the data as well as the cost for the “summary” of the node groups.

To minimize the total compression cost  $T$ , a two-step iterative approach is applied. Initially, the graph is considered as a single cluster itself. At each iteration, the algorithm first finds a good node grouping for a given number of clusters, and then, is looking for the number of clusters  $k$  to be formed by splitting the previously created clusters with the maximum entropy per node. This iterative procedure continues until finding the optimal number of clusters  $k$ , for which the compression cost  $T$  cannot further be decreased. Thus the complexity of the method is  $\mathcal{O}(Imk^2)$ , where  $I$  the number of iterations to achieve convergence of the compression cost (the author state that in practice  $I \leq 20$  iterations are enough). To conclude, the main features of the algorithm are: (i) it treats the community detection problem as a co-clustering task where the number of clusters is automatically determined by the MDL principle, and (ii) it scales linearly with respect to the number of edges.

#### 4.4.2. Probabilistic models and statistical inference

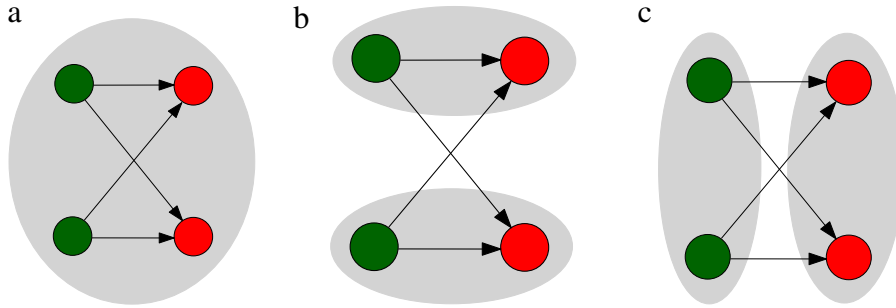
A different formulation and solution for the community detection problem in networks can be achieved applying statistical inference methods. Broadly speaking, statistical inference<sup>9</sup> is the process of drawing conclusions from data, subject to a set variables. Newman and Leicht [94] proposed an approach for community detection in directed networks based on mixture models for statistical inference. More precisely, let  $c$  be the number of communities in the network and assume that  $g_i$  represents the community (group) that node  $i$  belongs to. The group memberships are initially unknown and the goal of the algorithm is to infer them from the observed network structure. To this direction, the authors propose to use a mixture model<sup>10</sup> for the underlying communities and their properties, in which its parameters can be adjusted to find the best fit to the network. This point is particularly significant since the method does not assume any prior information about the network structure.

Assume that  $\pi_r$  is a variable that represents the fraction of nodes in community  $r$  and  $\theta_{ri}$  is the probability of existence of a directed edge from a particular node in community  $r$  to a node  $i$  (i.e., the preferences of nodes in  $r$  about which other nodes they link to). The following quantities are used to define the model: the network data  $\{A_{ij}\}$ , the missing data  $\{g_i\}$  (i.e., community assignment), and model parameters  $\{\pi_r\}$ ,  $\{\theta_{ri}\}$ . Defining a community as a set of nodes that have similar connection patterns to each other, the task of community detection can be formulated as a likelihood maximization problem. In this case, the goal is to maximize the likelihood  $\Pr(\mathbf{A}, g | \pi, \theta)$ , i.e., the probability that the data were generated by the given model, with respect to model's parameters. A common approach is to maximize the log-likelihood function instead of the

<sup>9</sup> Wikipedia's lemma for statistical inference: [http://en.wikipedia.org/wiki/Statistical\\_inference](http://en.wikipedia.org/wiki/Statistical_inference).

<sup>10</sup> Wikipedia's lemma for mixture models: [http://en.wikipedia.org/wiki/Mixture\\_model](http://en.wikipedia.org/wiki/Mixture_model).





**Fig. 12.** A simple case where the mixture model proposed by Newman and Leicht [94] has problem to assign the nodes of the network into communities (colors indicate community membership). The possible outputs of the method are those presented in the shadowed regions of (a) and (b), while the natural grouping presented in (c) cannot be identified (proposed by Ramasco and Mungan in Ref. [95]).

Source: Figure redesigned from Ref. [95].

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likelihood itself. At the end, the expected probabilities  $q_{ir}$  that node  $i$  belongs to community  $r$  can be expressed in terms of  $\{\pi_i\}$  and  $\{\theta_{ri}\}$  as

$$q_{ir} = \frac{\pi_r \prod_j \theta_{rj}^{A_{ij}}}{\sum_s \pi_s \prod_j \theta_{sj}^{A_{ij}}}. \quad (29)$$

Moreover, the authors state that the maximization of the likelihood occurs when

$$\pi_r = \frac{1}{n} \sum_i q_{ir}, \quad \theta_{rj} = \frac{\sum_i A_{ij} q_{ir}}{\sum_i k_i^{\text{out}} q_{ir}}, \quad (30)$$

where  $k_i^{\text{out}}$  is the out degree of node  $i$ . Combining Eqs. (29) and (30), an expectation–maximization (EM) algorithm can be applied to produce the belonging probabilities  $q_{ir}$  (the authors state that the convergence of the algorithm is fast).

As we mentioned earlier, the major strength of this approach is that it is independent from the underlying clustering structure of the network, making it capable to reveal various types of community structure. However, the number of communities is a parameter and needs to be specified a priori, but the authors state that it can also be inferred from the data.

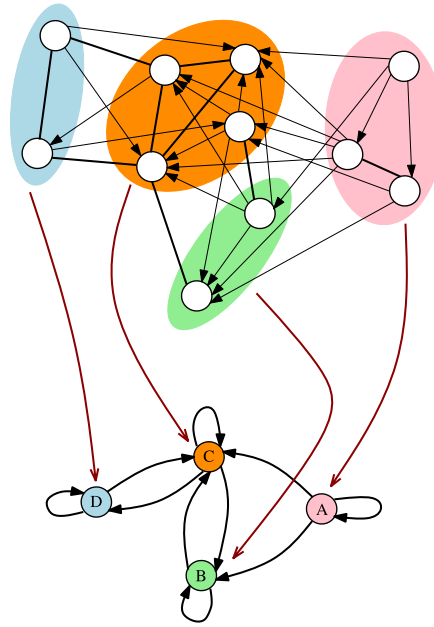
In a subsequent work, Ramasco and Mungan [95] observed that in the model of Newman and Leicht [94] that presented above, the probability  $\theta_{ri}$  that a node  $i$  has an incoming edge from a node in community  $r$ , suggests that each community  $r$  should have at least one node with non-zero out-degree. However, this constraint may have impact at the produced communities, as depicted in Fig. 12. In this case, the EM algorithm cannot identify the more natural and intuitive communities of a bipartite directed network, as shown in Fig. 12(c). On the other hand, the cluster assignments in Fig. 12 (a) and (b) are the possible outputs of the algorithm.

To avoid this problem, the authors of Ref. [95] generalize the EM approach, in such a way that the direction of edges do not restrict the possible assignment of nodes into groups. This can be achieved replacing the edge probabilities  $\theta_{ri}$  by three new types of probabilities: (i)  $\overrightarrow{\theta}_{ri}$  representing the probability of a directed edge from a node of community  $r$  to node  $i$ , (ii)  $\overleftarrow{\theta}_{ri}$  for the probability of having a directed edge from node  $i$  to a node inside community  $r$ , and (iii)  $\overleftrightarrow{\theta}_{ri}$  for a bidirectional edge between node  $i$  and a node in community  $r$ . Then, the problem is formulated according to the above new parameters and the generalized EM method is able to detect a broad range of diverse types of communities. Moreover, the authors provide a way for determining the number of communities in the EM formulation of the problem.

Another extension of the mixture models method by Newman and Leicht [94] has been presented by Wang and Lai [96]. The authors modified a subset of the parameters of mixture models, adding some interesting features to the proposed APBEMA algorithm, such as independence from the degree distribution of the network (i.e., there is no restriction about the degree of each node that affects the produced communities) and applicability to both directed and undirected networks without any modifications.

#### 4.4.3. Blockmodeling methods

*Blockmodeling* is an approach that has been extensively used to analyze and describe the structure of social networks and generally relational data (e.g., see Refs. [97–99]). The goal of blockmodeling is to represent a large and possibly incoherent network, by a smaller structure that can be interpreted more easily. In other words, blockmodeling can be considered as a clustering procedure, where the nodes of the network are grouped together according to how *equivalent* they are, under



**Fig. 13.** Schematic representation of a blockmodeling example [98]. The top graph corresponds to the initial directed network and the bottom one depicts how the network is represented by a blockmodeling approach.

Source: Figure redesigned from Ref. [98].

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some meaningful definition of equivalence. This procedure is similar to a reordering scheme of the adjacency matrix, causing the formation of a block-wise structure similar to the co-clustering task for community detection described in Section 4.4.1. Fig. 13 depicts an example where a blockmodeling approach has been applied in a directed network (top part of the figure), and how the network is finally represented (bottom part) [98]. That is, the corresponding blockmodel can be described by a matrix  $\mathbf{B}_{c \times c}$ , where  $B_{gq} = 1$  if an edge exists between groups (communities)  $g$  and  $q$ , and the goal is to find the node assignment into groups and the matrix  $\mathbf{B}$  that best fits the adjacency matrix  $\mathbf{A}$  of the graph.

Usually, two definitions of equivalence have been proposed: (i) structural equivalence, where the nodes are equivalent if they have the same connection patterns to the same neighbors, and (ii) regular equivalence, in which nodes are equivalent if they have the same or similar connection patterns to (possibly) different neighbors. Structural equivalence can be extended to probabilistic models, where the notion of stochastic equivalence is introduced: the nodes of the same group are said to be stochastically equivalent if their linking probabilities to any other node of the graph are the same. Holland et al. [100] describe the stochastic equivalence as “We say two nodes  $a$  and  $b$  are stochastically equivalent if and only if the probability of any event about the networks is unchanged by interchanging nodes  $a$  and  $b$ ”. The above definition is formed on the basis of the stochastic blockmodeling methods, in which every pair of nodes that belong to the same community are stochastically equivalent. In this case, every node belongs to a cluster and the relationships between different nodes are related to the corresponding pair of clusters (this is in contrast with more traditional mixture models, where nodes are assumed to be independent given their cluster assignments). Therefore, stochastic blockmodels can be considered as generative models for communities or blocks in networks and in the general case they fall in the class of random graph models. Finally, the problem is formulated as a maximum likelihood estimation. Wang and Wong [101] proposed a stochastic blockmodel for directed networks and applied it on small scale social networks. Another method for blockmodeling that can be applied on both directed and undirected networks (also in weighted networks), was presented by Reichardt and White [102].

Yang et al. [103] proposed a stochastic blockmodel for directed networks, called Popularity and Productivity Link model (PPL), which aims to model both incoming and outgoing links simultaneously. In order to achieve this goal, they introduce two latent variables, namely productivity and popularity, to explicitly capture outgoing and incoming edges respectively. That is, in the general case, PPL models the joint probability  $\Pr(i \rightarrow, j \leftarrow)$ , i.e., the probability that there exists a directed edge from node  $i$  to node  $j$ , as follows

$$\begin{aligned} \Pr(i \rightarrow, j \leftarrow) &= \sum_c \Pr(i \rightarrow | c) \Pr(j \leftarrow | c) \Pr(c) \\ &= \sum_c \left( \frac{\gamma_{ik} \alpha_i}{\sum_{i'} \gamma_{i'c} \alpha_{i'}} \frac{\gamma_{jk} \beta_j}{\sum_{j'} \gamma_{j'c} \beta_{j'}} \sum_{i'} \gamma_{i'c} w_{i'} \right), \end{aligned} \quad (31)$$

where  $\gamma_{ic}$  represents the probability of node  $i$  to belong to community  $c$ ,  $\alpha_i$  the productivity of node  $i$  (i.e., how likely an edge starts from  $i$ ),  $\beta_j$  the popularity of node  $j$  (i.e., how likely an edge is received by  $j$ ) and  $w_i$  the weight of node  $i$  for deciding the  $\Pr(c)$  that belongs to community  $c$ . A generative process can be defined for Eq. (31) and finally, through an EM algorithm the MLE solution can be derived (the complexity per iteration for the EM algorithm will be linear).

A limitation of the stochastic blockmodels is that each node belongs only to one community. However, this may not hold for several types of network data; in many cases nodes belong to more than one communities. Airoldi et al. [104] proposed the *mixed membership* model, an extension of the stochastic blockmodel, where each node belongs to any possible communities via a membership probability. That is, allowing multiple membership of nodes into communities, one is able to capture different underlying roles that nodes may exhibit in the network (similar to the concept of overlapping communities). More precisely, each node  $i$  is associated with a  $K$ -dimensional vector  $\vec{\pi}_i$ , where  $\pi_{i,g}$  denotes the probability that node  $i$  belongs to group (community)  $g$  and  $K$  is the number of groups. Moreover, for each pair of nodes  $i, j$ , the indicator vector  $\vec{z}_{i \rightarrow j}$  denotes the membership of node  $i$  regarding its interaction with node  $j$ , and  $\vec{z}_{j \rightarrow i}$  the group membership of node  $j$  regarding node  $i$ . Then, the mixed membership stochastic blockmodel for a graph  $G = (V, E)$  (directed) is drawn according to the following procedure:

- For each node  $i \in V$ :
  - Draw a  $K$ -dimensional mixed membership vector  $\vec{\pi}_i \sim \text{Dirichlet}(\vec{\alpha})$
- For each node pair  $(i, j) \in V \times V$ 
  - Draw membership indicator for  $\vec{z}_{i \rightarrow j} \sim \text{Multinomial}(\vec{\pi}_i)$
  - Draw membership indicator for  $\vec{z}_{j \rightarrow i} \sim \text{Multinomial}(\vec{\pi}_j)$
  - Sample the value of their interaction  $E(i, j) \sim \text{Bernoulli}(\vec{z}_{i \rightarrow j}^T \mathbf{B} \vec{z}_{j \rightarrow i})$

where matrix  $\mathbf{B}_{K \times K}$  represents the probabilities of interactions between different communities. The authors discuss how one can compute the parameters of the model, and they provide several experiments on real data (e.g., social networks, protein interaction data).

A different kind of blockmodel was recently presented by Rohe and Yu [105], and is based on the notion of co-clustering (i.e., the task in which both rows and columns of the adjacency matrix are clustered simultaneously). The blockmodel is also accompanied by a new spectral clustering algorithm for directed networks. More precisely, at a first step a new co-clustering algorithm for directed networks is introduced, based on the decomposition of a graph's Laplacian defined by the authors. The idea behind this approach is based on the fact that the co-clustering task may be more meaningful for the case of directed networks: two rows will belong to the same co-cluster if they have common endpoints, while two columns will be in the same co-cluster if they receive edges from several common nodes. The authors extend the spectral clustering algorithm presented in Section 4.3.2 (either for directed or undirected networks) to the co-clustering task, where the eigendecomposition is replaced by the singular value decomposition for dealing with the asymmetric matrix. To better understand the properties of the algorithm, the authors present a stochastic blockmodel for directed networks, based on the concept of co-clustering. That is, the notion of stochastic equivalence is relaxed into two types, in order to capture the two different roles of nodes (senders and receivers):

- Two nodes  $i$  and  $j$  are stochastically equivalent senders if and only if  $\Pr(i \rightarrow v) = \Pr(j \rightarrow v)$ ,  $\forall v \in V$ .
- Two nodes  $i$  and  $j$  are stochastically equivalent receivers if and only if  $\Pr(v \rightarrow i) = \Pr(v \rightarrow j)$ ,  $\forall v \in V$ .

In the case of blockmodels for the traditional clustering task, both these conditions for stochastic equivalence should occur. On the other hand, considering these concrete cases of stochastic equivalence, a blockmodeling based notion of co-clusters can be defined. The authors define formally the *stochastic co-blockmodel* for directed networks and study thoroughly the performance of their spectral algorithm under this model.

#### 4.4.4. Other approaches

In this section we describe diverse approaches that can generally be applied in the task of community detection and exploration in directed networks. In most cases, these methods adopt completely different methodological approaches and they typically deal with variations of the community detection problem (e.g., community detection for time evolving networks or community exploration methods). Some of these topics will also be discussed in Section 8, since they constitute interesting extensions and future research directions for the problem.

#### Community structure exploration and evaluation methods

**Community kernels.** Most of the approaches presented so far are based on the assumption that communities correspond to subgraphs with dense internal connections and sparse external connections, while there is no special treatment of the most influential nodes of the network. However, in many cases (usually in social networks), there exist some influential nodes (e.g., important/popular users in online social networking applications such as twitter) whose community structure is quite different from that of the other nodes. To deal with these cases, Wang et al. [106] proposed the notion of *community kernels* and studied the problem of community kernel detection in social networks (both directed and undirected), as a way for exploring the community structure of large networks. Usually, social networks (e.g., Twitter's who-follows-whom network) form a near bipartite structure, where one partition corresponds to a few influential nodes (e.g., celebrities or politicians)

while the other to the rest of the nodes; the partitions are typically connected via a large number of edges targeting to influential nodes, as shown in the leftmost part of Fig. 14. Most of the well known community detection algorithms (which are based on density-based measures) cannot identify this underlying structure, partitioning the influential users into different communities and placing them in the same communities with their followers (Fig. 14 (center)). However, one would expect that the influential nodes should be placed in the same communities according to common interests (e.g., politicians, entertainers) forming the community kernels, while for each kernel there should exist a corresponding auxiliary community that is associated with that kernel (rightmost part of Fig. 14).

Wang et al. [106], at a first step defined the notion of community kernel; each member of the kernel has more connections with members of the same kernel, than outside of it. Moreover, each member (node) of an auxiliary community has more connections with the associated kernel than to any other kernel. The notion of community kernels can also be applied in several settings. For example, in a co-authorship network, a kernel may correspond to a group of senior researchers or professors in a specific area, while the auxiliary community to a group of students or junior researchers in this area. Two algorithms are proposed to extract the community kernels of large scale social networks, a greedy one and WeBA which provides approximation guarantees (since the problem of identifying the best community kernel is computationally difficult). Both of them scale linearly with respect to the size of the network.

**Mutuality-tendency aware community detection.** Most of the approaches presented so far do not explicitly distinguish the existence of mutual (i.e., two nodes  $u, v$  are mutually connected if both directed edges  $(u, v)$ ,  $(v, u)$  exist in the network) or one-way connections between the nodes of a directed network in the graph clustering task. In other words, by simply minimizing the number of inter-cluster edges, clustering methods do not capture the existence of possible tendencies between node pairs to be mutually connected. This point is of particular interest since the existence of mutual connections in a cluster may be an indicator of cluster's stability. Towards this direction, Li et al. [107] developed a spectral clustering algorithm for directed networks, which takes into account the tendencies of node pairs to form reciprocal (mutual) connections. More precisely, the mutuality tendency among a pair of nodes is quantified using graph theoretic concepts and according to this, a mutuality tendency aware criterion for the clustering algorithm can be defined by maximizing the intra-cluster mutuality tendency and minimizing the inter-cluster mutuality tendency. Fig. 15 depicts an example of a social network where nodes of the same group tend to have reciprocal connections, while nodes across different groups are connected by one way edges. When applying traditional spectral clustering methods (Fig. 15 (a)), the nodes of the second group (Group B) are partitioned into two clusters, while a tendency aware clustering approach (Fig. 15 (b)) is able to utilize edges' mutuality information and thus the majority of mutual connections are placed within the same clusters [107].

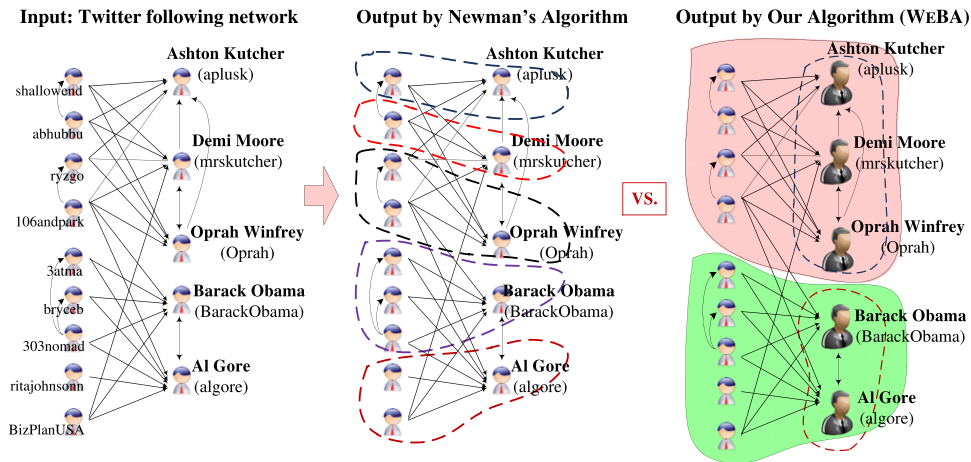
**Connected components based method.** A simpler explanation about the notion of communities is given in Ref. [108]. The authors argue that a specific type of connected components in the network, can be used to represent and explore the community structure. Generally, the definition of connected components in directed networks is more complicated than the undirected case, and the main types are the following: weakly connected component (WCC), connected component (or unilaterally connected component - UCC) and strongly connected component (SCC) (see Section 2 for details). The authors of Ref. [108] applied a more strict definition and more precisely the one of strongly  $p$ -connected components ( $p$ -SCC). A  $p$ -SCC corresponds to a subgraph  $G' = (V', E')$ , in which  $\forall u, v \in V'$ , there is a directed path of length at most  $p$  between  $u$  and  $v$  and one between  $v$  and  $u$ , with  $p \geq 2$ . In other words, the notion of  $p$ -SCC represents a SCC with an additional constraint on the path length between two nodes. The authors combined the  $p$ -SCC concept with a merging routine that adjusts the size of the produced communities, to detect clusters in directed networks.

**Core-based community exploration.** The notion of community structure is also closely related to the one of collaboration between the nodes of a network. A natural mechanism for the formation of a community in networks is related to the notion of cohesion, which actually quantifies the collaboration nature among its members. In other words, quantifying the degree of cohesion of a community, one can estimate the collaboration among its elements. To the direction, Giatsidis et al. [109] introduced novel metrics for evaluating the cohesion of directed networks, extending the  $k$ -core concept from the undirected setting to the one of  $D$ -cores for directed networks. Broadly speaking, a core can be defined as a maximum size subgraph that is dense enough, i.e., for each node in the subgraph, there exist at least  $k$  incident edges that are adjacent to nodes of the same subgraph. The concept is extended to directed networks, where the  $(k, \ell)$ - $D$ -core is defined, which corresponds to a maximal size subgraph where for every node  $i$  in the core,  $k_i^{in} \geq k$  and  $k_i^{out} \geq \ell$  (the in- and out-degree respectively), leading to a degeneracy-based community exploration and evaluation approach.

**Game-theoretic approaches.** A different formulation of the clustering and community detection task in directed networks can be achieved based on game-theoretic notions. Torsello et al. [110] presented a framework for clustering in directed networks within the context of object grouping in computer vision and pattern recognition. The grouping process is expressed as a non-cooperative game of the competition between the hypotheses of group membership, where groups (clusters) correspond to evolutionary stable strategies.

#### Extracting the best clusters on large scale directed networks

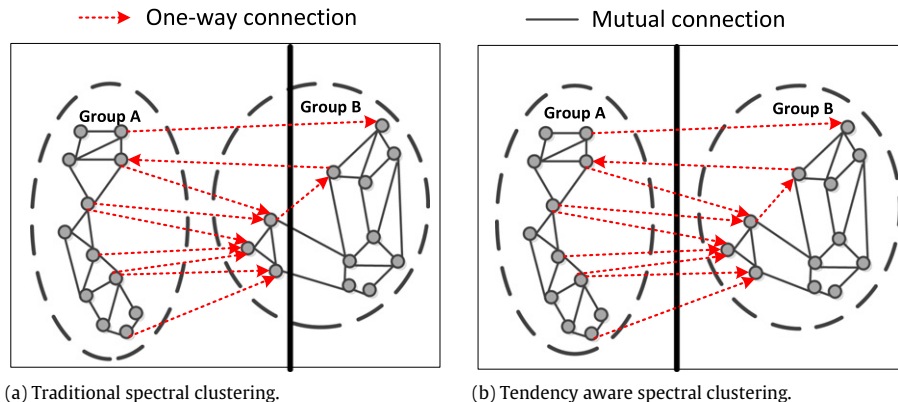
An important characteristic of real networks which recently has gained an increased interest is their size (scale). As networks grow in size, the complexity of the analysis tasks applied to them (including the clustering/community detection



**Fig. 14.** An example of community kernel detection (rightmost figure) in the Twitter network (leftmost figure) and how the outcome is differentiated from a traditional community detection method based on modularity (central figure) [106].

Source: The figure is courtesy of Wang et al. [106].

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**Fig. 15.** An example of the difference between traditional spectral graph clustering (a) and tendency aware spectral clustering (b) defined by Li et al. [107]. The dashed line edges represent one way edges while normal lines show mutual connections.

Source: The figure is courtesy of Li et al. [107].

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task) increases, and therefore the feature of scalability should be taken into consideration. Moreover, regarding the graph clustering task, many applications require only a subset of the “best” clusters and not all the possible clusters produced by an algorithm. In other words, depending on the application domain, not all possible clusters of the entire graph are useful, but the most strongly connected ones are typically needed. For example, in a social networking application, only the most strongly connected groups of individuals may be of interest. Methods that first identify all the clusters of a network, rank them and keep only the top clusters tend to be inefficient, both in time and space requirements. However, it is possible to reduce the searching space of an algorithm by a pruning process, examining only those clusters with the highest scores (regarding their quality).

Macropol and Singh [111] proposed the TopGC (Top Graph Clusters) algorithm, for finding the best connected, clique-like clusters in large networks. The algorithm works on both directed and undirected networks finding variable size clusters, while its running time is linear with respect to the size of the network. The basic idea behind the algorithm is based on the observation that nodes with similar neighbors in a graph, generally should belong on the same cluster. In other words, the overlap between the neighbor sets for two nodes is an indicator for whether or not these nodes should be clustered together (e.g., the neighbor sets of the nodes of a clique (except from the node itself) match exactly). The TopGC algorithm exploits the fast similarity search based on *Locality Sensitive Hashing* (LSH) in order to find nodes with similar neighborhoods. In addition, the LSH method is modified to achieve reduced memory consumption, since only the best clusters of the graphs need to be extracted. The authors also state that the algorithm is highly parallelizable, making its implementation possible in the MapReduce framework [112].



### Dynamic networks

One important aspect of several real-world networks is their dynamic nature, i.e., they are not static but typically evolve over time with the addition/deletion of nodes/edges, forming graph streams. A graph stream  $\mathcal{G}$  is defined as a sequence of graphs  $G^{(t)}$ , i.e.,  $\mathcal{G} := \{G^{(1)}, G^{(2)}, \dots, G^{(t)}, \dots\}$  [113]. Dynamic networks have recently gained much attention from the research community due to their interesting structural properties (e.g., Refs. [114,115]). Regarding the graph clustering and community detection problem, the works presented so far in this paper mostly concern with the problem applied on static directed networks. In other words, we are interested to extract the community structure of the network at a specific time point  $t$  of its evolution, working on the snapshot  $G^{(t)}$  of the network at timestamp  $t$ . However, an interesting question is how the problem of community detection can be extended and tackled in the case of dynamic networks. In this case, we need approaches that will be able to incrementally find communities on networks, as well as to monitor and detect changes in the community structure over time. Thus, two sub-problems need to be addressed:

- (a) *Community discovery*: Node assignment into clusters (communities), following any of the definitions presented in Section 3.
- (b) *Change point detection*: How to quantify and detect the change of the community structure over time?

More precisely, the community detection problem in dynamic networks can be treated as a two-step incremental procedure: (a) the community discovery subtask refers to static snapshots of the time-evolving graph, while (b), in the change detection subtask, a measure of similarity between different partitions over time needs to be determined in order to detect change points in the graph stream. These change points correspond to time points where a significant change in the already identified community structure has occurred. The above problem has been studied for both undirected [113] and directed networks. In the latter case, the authors of Ref. [116] present an approach for detecting the community structure and the change points in dynamic weighted directed networks. The first subtask is achieved by applying the method of Random Walks with Restart [117] (for computing the relevance scores of the nodes), combined with a local version of modularity for examining the quality of the produced partition. For the change detection subtask, the authors propose a similarity metric between partitions, in order to detect change points over time, accompanied by an algorithm for updating the partition of a graph segment when a new graph is added on the stream.

## 5. Definition-based classification of clustering methods

In Section 4 we presented our main classification for the clustering approaches in directed networks, targeting methodologies and algorithms that have been presented so far for the problem. In this section, we consider a different but also important (and in some cases supplementary) classification scheme, where the methods are grouped according to the clustering notion they adopt.

In Section 3 we discussed the two main clustering notions in directed networks, otherwise the two main approaches to characterize a subset of nodes as a cluster. The first and most common one, namely *density-based clusters*, is based on the concept of intra-cluster and inter-cluster edge density (see Section 3.1 for more details). That is, a cluster is considered to be a subgraph with high internal edge density and low external one. Depending on the objective measure that is used to quantify edge density, some variations of the general intra- and inter-density measures can be considered (e.g., considering only the intra-cluster edge density of a subgraph). Nevertheless, in all these cases, the feature that dominates on the characterization of a cluster is expressed as a function of edge density.

The second clustering notion in directed networks is more broad and includes cases where nodes are clustered together based on criteria beyond the classical one of edge density – see Section 3.2 for a more detailed description. That is, in several cases, the presence of (directed) edges create interesting structures that deviate from the well-known density rule and can be naturally considered as clusters. Examples of pattern-based clusters are the ones presented in Fig. 3. It is clear that these clusters represent a variety of interesting patterns (e.g., citation-based clusters or the case where the cluster represent a subgraph that imposes “strong” information flow). Furthermore, as we will present shortly, in most cases the notion of pattern-based clusters co-exist in a network with the one of density-based. That is, a large number of methods is able to group the nodes of a network following a density rule combined by other more sophisticated types of structural patterns, that the “pure” density-based approaches are not able to distinguish. To conclude, one can say that both types of clusters represent diverse and interesting structures and patterns, that induced by the edges of the networks (link-density for the former case and link-pattern for the latter one [51]).

The goal of this section is to provide a categorization of the approaches reviewed in Section 4 according to their clustering type-notion. A summary of this classification with the most representative algorithms is also presented in Table 2. Since density-based and pattern-based clusters may co-exist on a directed network, we also provide a discussion on these cases.

### 5.1. Density-based clusters

In this category of “pure” density-based clustering, usually belong approaches that become well-known extensions from the undirected case. That is, spectral clustering methods based on the directed Laplacian matrix [75,61,76,105] are examples of approaches that identify density-based clusters. The graph clustering method based on the weighted cuts criterion (proposed by Meilă and Pentney [59]), also leads to similar clustering results. The attraction and repulsion approach

**Table 2**

Summary of the basic graph clustering approaches for directed networks. The field of Category represents one of the three main categories presented in Section 4 (excluding the naive approach): 1st: transformations maintaining directionality, 2nd: extending objective functions and methodologies to directed networks, 3rd: alternative approaches. The type (notion) of clusters that identified by the methods is also depicted. The fourth column shows the objective function applied by each method (in case where an objective function is clearly described), while the next column presents some additional features of the methods. The last column describes the time complexity of each method (more generally the factors that determine the complexity). Typically, the complexity of spectral optimization (Spectral Opt.) relies on the complexity of eigenvalue decomposition (spectral decomposition).

Method	Category	Clustering type	Objective function	Additional features	Complexity
Symmetrization [54]	1st	All			$\mathcal{O}(\sum_i \mathbf{D}(i))$
Network embedding [56]	1st, 2nd	All	Directed modularity	Laplacian matrix	Selected algorithm
Random walk sim [64]	1st	All			Selected algorithm
Bipartite modularity [66]	1st, 2nd	All	Bipartite modularity	Directed to bipartite	Modularity opt.
MAGA method [67]	1st, 2nd	All	Bipartite modularity	Genetic algorithm (GA)	Complexity of GA
Semi-supervised learning [57]	1st, 2nd	All	Modified modularity		Spectral opt.
Directed modularity [50,58]	1st, 2nd	All	Directed modularity		Spectral opt.
LinkRank [55]	2nd	All	Directed modularity		Modularity opt.
DGRN [70,71]	2nd	All	Directed modularity		Spectral opt.
Overlapping modularity [73]	2nd	Density-based	Dir.-Overl. modularity	Genetic algorithm	$\mathcal{O}( C n^2)$
Local modularity [74]	2nd	Local cohesive groups	Local modularity		Modularity opt.
Directed Laplacian [75]	2nd	Density-based	Normalized cuts		Spectral opt.
Directed normalized Laplacian [61]	2nd	Density-based	Normalized cuts		Spectral opt.
Multiple views spectral clus. [76]	2nd	Density-based	Multiple cuts	Multiple views	Spectral opt.
Weighted cuts [59]	2nd	Density-based	Weighted cuts		Spectral opt.
Attraction and repulsion [77]	1st, 2nd	Density-based	Normalized cuts		Spectral opt.
Two-step random walks [82]	2nd	All	Normalized cuts		Spectral opt.
Local partitioning [87]	2nd	Density-based	Conductance	Local method	Spectral opt.
Message passing [85]	2nd	All		Affinity propagation	$\mathcal{O}(\ln C  + 2n^2)$
Directed clique percolation [88]	2nd	Density-based	$k$ -clique		$\mathcal{O}(\exp(n))$
Local density [89,90]	2nd	Density-based	Density	Local method	
Infomap [18]	3rd	Pattern-based	Code length	Compression	Optimization method
AutoPart [93]	3rd	Density-based	Code length	Compression	$\mathcal{O}(m C ^2)$
Mixture models [94–96]	3rd	All		Mixture models, EM	Convergence of EM
Blockmodels [101,103,102,104]	3rd	Density-based			Parameter estimation
Co-Blockmodel [105]	3rd	Density-based		Spectral	Spectral decomposition
Community Kernels [106]	3rd	All		Kernel's Score	Linear approximation

of Ref. [77] proposed in the field of image analysis and computer vision, also belongs to this category, as it constitutes a generalization of the normalized cuts criterion for directed networks. Furthermore, this category includes the local partitioning [87] and local density methods [89,90]. Other approaches that based solely on the density-based notion of clusters are the co-clustering algorithm (AutoPart) presented in Ref. [93], the directed clique percolation method [88] and techniques based on the blockmodeling concept for statistical inference [101,103,102,104].

## 5.2. Pattern-based clusters

The second category of methods are those based on the concept of pattern-based clusters, i.e., clusters beyond the edge density notion. One interesting thing is that most of these methods are able to identify a mixed type of density-based and pattern-based clusters. In other words, they still identify clusters based on the density concept, however they enhance these clusters with other significant patterns. For example, using the idea of graph symmetrization [54], one can transform the directed network into an undirected one using measures that capture the incoming and outgoing edge similarity, leading to the concept of citation-based clusters (see Fig. 3(a), (b)). In other words, the graph is transformed to an undirected one using nodes' incoming and outgoing edge similarity, and therefore at the clustering process it is possible two nodes to belong on the same cluster even if they are not directly connected in the original directed network. This constitutes an important feature, especially for the case of networks where such underlying information exists (e.g., citation networks).

The directed version of modularity presented by Arenas et al. [58] and Leicht and Newman [50], has formed the basis for several community detection approaches in directed networks. It is able to extract density-based clusters, but it also has the ability to recognize significant patterns imposed by edge directionality: it can classify the nodes of a network into clusters, in such a way that directed edges link from the one cluster to the other. Furthermore, similar behavior can be observed even in networks with no underlying community structure; this is an additional evidence that directed edges lead to various interesting underlying patterns. However, as we presented in Section 4.3.1, the above version of modularity has the drawback that it cannot distinguish properly the direction of edges (see Fig. 9).

Another interesting type of pattern-based clusters is the one presented by Rosvall and Bergstrom [18] and is based on the concept of patterns of movement among the nodes of a directed network. The community detection method presented

in that work (Infomap) is based on random walks and the main intuition is that a community can be defined as a group of nodes where the random surfer is more likely to be trapped in. This concept can be treated as an increased flow circulation pattern between the nodes of the same community, as presented in Fig. 3(c). Several community detection approaches for directed networks have also been built upon this flow-based pattern. Lai et al. [56] presented a Laplacian network embedding algorithm which apart from density-based clusters, it is able to detect flow patterns among the nodes. Their subsequent approaches based on random walk similarity [64] and affinity propagation [85], are moving in a similar axis. The LinkRank method introduced by Kim et al. [55] is also able to extract flow-based patterns. Moreover, as discussed in the paper, their generalized version of modularity can distinguish in a proper way the direction of the edges, compared to the one of Leicht and Newman [50]. Additionally, the approaches that utilize the Directed Gaussian Random Network (DGRN) as null model [70,71], are also able to cluster the nodes of directed networks based on information flow patterns.

In the approach of Guimerà et al. [66], the directed network is converted into a bipartite one, and a bipartite version of modularity is applied to extract the community structure. While the method mainly considers density features, it is also able to detect communities based on common incoming and outgoing edges; it relies on the idea of actors co-participation in a team (for bipartite networks). Additionally, other methods that consider the directed network as a bipartite one, are also able to detect both density-based as well as citation-based clusters [57,67]. A similar behavior is presented in the two-step random walks method by Huang et al. [82]; the two-step random walk model is able to capture important connectivity patterns by exploiting the existence of co-citation and co-reference relationships.

The method of Newman and Leicht [94] based on mixture models can detect diverse types of clusters, including assortative<sup>11</sup> and disassortative structures. However, as discussed in Section 4.4.2, the method cannot identify communities that do not have at least one node with non-zero out-degree (see Fig. 12). The approach of Ramasco and Mungan [95] and Wang and Lai [96] overcomes this problem, recovering clusters that do not necessarily follow the density-based notion.

### 5.3. Empirical comparison of clustering approaches in directed networks

Having reviewed the methods proposed so far for the clustering problem in directed networks, we will now proceed with a brief empirical comparison of them. Table 2 presents a summary of the major approaches along with their basic features.

As we discussed earlier, the proposed approaches follow diverse methodologies and in many cases they are built upon different notions of clusters/communities in directed networks. In the first case which follows naturally from the problem in undirected networks, only density features are considered to characterize a cluster. Typically, the edges between nodes of the network represent pairwise relationships, which operate as similarity measure among different entities (nodes). However, as several research works propose, due to the existence of directed edges in a network, it is possible to exist other interesting type of clusters. In many cases, the proposed approaches are able to identify density-based clusters combined with interesting structures beyond the density pattern. For example, applying symmetrization schemes in the directed network, it is possible to group nodes in the same cluster, even if they do not share an edge in the initial network [54]. This constitutes an important characteristic for a set of networks where co-citation and co-reference relationships may be of interest (e.g., citation networks). Similarly, another interesting clustering definition is the one that based on random walks and the concept of information flow and movement among the nodes of a network (e.g., Ref. [18]).

A natural question that arises from the above discussion is which method should a researcher or a practitioner use. The answer is not clear but mainly depends on the network under consideration and on the application domain (for the latter we discuss in Section 7). In case of networks where edges represent pairwise relationships, it may be more useful to apply density-based methods or methods that, at least, are able to identify density-based clusters (e.g., modularity optimization, spectral clustering, etc.). On the other hand, when edges represent patterns of movement among nodes or generally some kind of information flow, methods that are able to recover flow-based clusters may be preferable.

Although the clustering notion–definition is an important feature for selecting a community detection method for directed networks, it is not the only one. As we discussed in previous sections, there exist a plethora of algorithms that seems to follow the same clustering definition. For these approaches, additional features should be compared in order to select the most suitable one for a specific application or for a specific graph dataset that needs to be analyzed. Some important features are the ones presented in Table 2. For example, one may select an appropriate algorithm examining the objective function that is used to characterize the quality of a community (e.g., modularity, normalized cuts). Some methods pose additional characteristics, such that their ability to identify overlapping communities, that may be significant for specific applications. The time complexity of an algorithm is also a crucial factor, especially for large scale networks. Since in most cases the clustering problem is expressed as an optimization one, the complexity depends heavily on the selected optimization method [11].

Thus, it becomes clear that selecting the proper clustering approach depends on multiple criteria. In Section 7 we will see which of these approaches have been used in the related literature for specific applications in several domains. This may be useful for practitioners without the required know-how in the field.

<sup>11</sup> Assortativity is the property where the nodes of a network tend to link to other nodes that are similar in some way (see Wikipedia's lemma for Assortativity: <http://en.wikipedia.org/wiki/Assortativity>).

## 6. Evaluation metrics and benchmarking

In this section we discuss on the task of assessing the results of a graph clustering algorithm. Generally, a network can be divided into several meaningful partitions and one should decide which of them is the most appropriate as a clustering result. Typically, quality measures are used for this task, but in some cases, their accuracy may not be a good indicator [11]. Moreover, since a wealth of diverse algorithms has been proposed for both directed and undirected networks, one wants to decide which algorithm results in better performance — in terms of clustering quality; of course, the performance of an algorithm in terms of time complexity is also a crucial factor. In other words, an important problem in the area is the one of evaluating the performance of clustering algorithms by comparing their results. In the case where real datasets with known community structure (ground truth) are available, this can be done by comparing the results with the a priori known node assignments to communities/clusters. Moreover, a widely applied approach is to evaluate the performance of a community detection algorithm on benchmark graphs with an inherent community structure. However, in the case of directed networks both techniques are still premature. On the one hand, it is very difficult to find directed graph datasets with known community structure and sufficient size, while only a few benchmark graphs exist.

The directed clustering evaluation task is closely related to the respective one in the undirected case and a more thorough discussion is presented in Refs. [11,19]. In the case of quality measures, typically the directed version of modularity [58,50] is applied to quantify the significance of a partition, while for benchmarking purposes some very recent benchmarks are reviewed.

### 6.1. Evaluating partitions

The problem of evaluating the quality of communities produced by an algorithm is rather broad and several approaches have been proposed and applied in the undirected case of the problem. Most of them are applied directly to the clustering problem in directed networks, since the algorithms and the results for both problems can be treated similarly. An approach is to examine quality indices for partitions in directed networks, and some of them were presented in Section 4 (e.g., modularity). As noted by Schaeffer [19], although the optimization process of these measures is a difficult issue, their evaluation for a given partition of the network is a more lightweight operation. However, the evaluation process may be biased regarding the characteristics of the quality measure. Moreover, while there are several comparative studies on quality measures for undirected graph clustering [118,39], similar studies are missing for the directed version of the problem.

An alternative approach to evaluate the produced clusters is related to the stability of the results under perturbations of the input graph. The motivating idea behind this technique is the following: if a cluster is significant, then after some modifications at the original network, its significance will be retained and the cluster itself will be still identified by the algorithm. Typically, the stability of an algorithm is examined by measuring the number of operations needed to transform the original clustering results to the ones produced after the perturbation of the graph. In the related literature different perturbation approaches have been proposed for undirected networks [119–121], but their applicability to directed ones is not straightforward. (For a more detailed presentation one can refer to Ref. [11].)

### 6.2. Comparing algorithms

Instead of examining the quality of the clustering results produced by an algorithm, it may be preferable to compare the results produced by several algorithms, towards selecting the most accurate one. For this task, one has to define a similarity criterion between results produced by different algorithms. In the case where a true assignment of nodes into clusters is known a priori (also known as ground truth clustering), these criteria can be used to evaluate the performance of a clustering algorithm. More precisely, suppose that  $C_A(v), \forall v \in V$  represents the cluster assignment of node  $v$  using algorithm  $A$ . Then, a similarity measure for two algorithms  $A, B$  with node cluster assignments  $C_A(1), C_A(2), \dots, C_A(n)$  and  $C_B(1), C_B(2), \dots, C_B(n)$ , can be defined as

$$S(A, B) = \frac{1}{n} \sum_{v \in V} \frac{|C_A(v) \cap C_B(v)|}{|C_A(v) \cup C_B(v)|}, \quad (32)$$

where a score value close to one indicates similarity for the clustering results. However, this measure does not behave well if the results of the one algorithm have been produced by a merging process of two or more clusters of the other algorithm [19].

In a similar spirit, one can use the measures of *precision* and *recall*, with respect to the ground truth clustering assignment. Suppose that  $\mathcal{C} = \{C_1, C_2, \dots, C_K\}$  is the output of a clustering algorithm, where  $K$  represents the number of clusters and  $C_j$  is the ground truth clustering. Then, for any output cluster  $C_i$  the precision and recall of this cluster can be defined as

$$\text{Prec}(C_i, C_j) = \frac{|C_i \cap C_j|}{|C_i|} \quad \text{and} \quad \text{Rec}(C_i, C_j) = \frac{|C_i \cap C_j|}{|C_j|}. \quad (33)$$

A measure that integrates precision and recall is the so-called *F-measure*  $F(C_i, C_j)$  defined as the harmonic mean of precision and recall<sup>12</sup>:

$$F(C_i, C_j) = \frac{2 \cdot \text{Prec}(C_i, C_j) \cdot \text{Rec}(C_i, C_j)}{\text{Prec}(C_i, C_j) + \text{Rec}(C_i, C_j)}. \quad (34)$$

Each produced cluster  $C_i$  is matched with its corresponding ground truth cluster  $C_j$  for which the F-measure is maximized,  $F(C_i) = \max_j F(C_i, C_j)$ . Then, the average F-measure of the produced clustering is defined as the average F-measure over the set of clusters as

$$F(\mathcal{C}) = \frac{\sum_i |C_i| \cdot F(C_i)}{\sum_i |C_i|}. \quad (35)$$

Another important category of similarity measures for assessing the results of clustering algorithms, originates from the field of information theory. Danon et al. [21] used the measure of *Normalized Mutual Information* (NMI), which considers information-theoretic concepts and is based on the fact that if two clusters are similar to each other, then only a small amount of additional information is needed to infer one clustering assignment from the other. The definition is based on the concept of confusion matrix  $\mathbf{N}$  (the rows correspond to the ground truth clusters while the columns to the clusters identified by the algorithm), and it can be expressed as follows

$$\text{NMI}(A, B) = \frac{-2 \sum_{i=1}^{C_A} \sum_{j=1}^{C_B} N_{ij} \log \left( \frac{N_{ij} N}{N_i N_j} \right)}{\sum_{i=1}^{C_A} N_i \log \left( \frac{N_i}{N} \right) + \sum_{j=1}^{C_B} N_j \log \left( \frac{N_j}{N} \right)}, \quad (36)$$

where  $|C_A|, |C_B|$  represent the number of ground truth clusters and the number of produced clusters respectively. The element  $N_{ij}$  corresponds to the number of nodes in real cluster  $i$  that appear in the produced cluster  $j$ , while  $N_i$  is the sum over row  $i$  and  $N_j$  the sum over column  $j$  of the confusion matrix  $\mathbf{N}$ . In the case where the produced results are identical with the ground truth, the NMI( $A, B$ ) measure takes its maximum value one, while in the case where the two clusterings totally disagree, the NMI( $A, B$ ) score is zero. Using information-theoretic concepts, the numerator of Eq. (36) corresponds to the mutual information between the two clustering results, while the denominator represents the sum of the corresponding entropies (actually the mutual information and entropies of the random variables that represent the cluster assignments). We also stress here that these measures can also be applied to compare two clustering assignments and not necessarily a comparison to ground truth data. Other information-theoretic criteria for comparing different clustering results have been presented by Meilă [122] (see the related paper by Fortunato [11] for more details).

### 6.3. Testing algorithms

The step that follows the design of a new community detection algorithm, involves the testing process. Usually, in this task, the algorithm is applied to a network with specific community structure and the results are compared to the known structure. To do this, the algorithm should be applied to a network with well defined community structure, in order to extract meaningful conclusions about its function. For this reason, the use of benchmark graph datasets is involved. In the case of undirected networks, there exist a few real graphs with known community structure that are commonly used for testing community detection algorithms. The most known of them is Zachary's social network (see e.g., Ref. [41]), which represents friendship relationships between the members of a karate club. However, in most cases, these graph datasets are of small scale and they are not adequate for testing the performance (in terms of accuracy) of an algorithm at larger scale. Moreover, for the directed graph clustering problem, there does not exist any such commonly used set of benchmark graphs that can be used to assess the accuracy of algorithms.

A similar way to test a graph clustering algorithm is to examine its performance on synthetic benchmark graphs, i.e., computer generated graphs with built-in community structure. These graphs are artificial and typically produced by a mechanism which is controlled by some parameters. Several benchmark graph datasets have been proposed for the undirected graph clustering problem, such as the *planted  $\ell$ -partition model* and the *LFR benchmark* (see Ref. [11] for more details). For the case of directed networks which is the focus of this paper, the problem of generating realistic benchmarks has received relatively little attention from the research community. In several research works where a new algorithm is proposed, some specific benchmark directed graph datasets are also presented and used for testing the algorithm. For example, Rosvall and Bergstrom [18] proposed the directed network presented in Fig. 3(c) as a benchmark for clustering algorithms that consider flow-based types of clusters (similar synthetic benchmarks have been also presented in other research works).

<sup>12</sup> Wikipedia's lemma for precision, recall and F-measure: [http://en.wikipedia.org/wiki/Precision\\_and\\_recall](http://en.wikipedia.org/wiki/Precision_and_recall).



Recently, Lancichinetti and Fortunato [123] presented an algorithm for generating directed graph benchmarks for testing purposes (the generator has also the ability to produce weighted graphs with overlapping communities). The benchmark graphs constitute an extension of the LFR undirected graph generator and consider that the in-degree  $\{y_i\}$  and out-degree  $\{z_i\}$  sequences follow some specific distributions. Moreover, the size of the produced communities follow a power-law distribution. The generation mechanism is as follows: initially, we sample the in-degree sequence  $\{y_i\}$  from a power-law distribution, and the out-degree sequence  $\{z_i\}$  from a  $\delta$  distribution (by drawing  $N$  random numbers for each of them). Each node in the graph shares some of its edges with other nodes inside its community and the rest of the neighbors are outside the community depending on its degree (in- and out-). For this reason, two topological mixing parameters are introduced for each node, to define the proportion of incoming and outgoing edges that will fall inside and outside node's community. According to these parameters, nodes of the same community (stubs) are randomly connected (preserving both in-degree and out-degree distributions) and some extra random edges are placed between them and nodes of different communities.

The LFR benchmark graphs are constructed based on a density rule, which places internal and external edges between nodes of the same and of different communities respectively. However, as we have already seen throughout this survey paper, the existence of directed edges may reflect other interesting structural patterns, such as the flow-based pattern. From a first view it seems that the LFR generator is not suitable to generate graphs with patterns of flow between nodes. However, as the authors discuss, this can be achieved by constraining the number of incoming and outgoing edges of communities.

## 7. Real-world applications on directed networks

The task of graph clustering and community detection in general, and the one of directed graph clustering in particular, lies at the heart of many applications and research agendas. A large number of research works in several scientific disciplines have been devoted to increase our understanding of real-world complex systems, applying graph clustering approaches. In this section we review some important applications of the clustering problem in directed networks, in several fields, such as social and information sciences, biology, and neuroscience. Since the clustering task constitutes one of the most common and prominent analysis tool in networks, the following list of possible applications can be extended in every other field where directed networks appear.

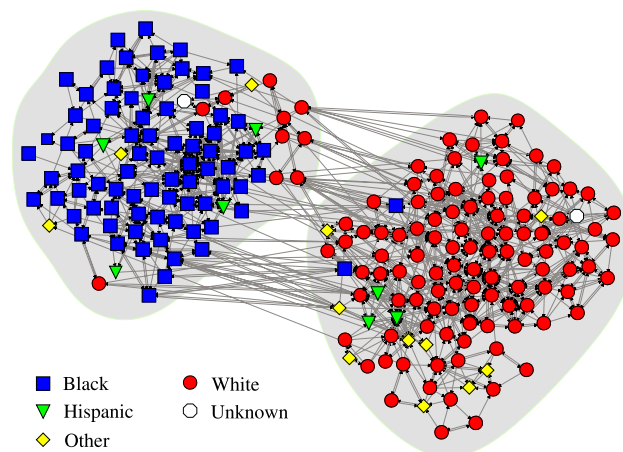
### 7.1. Social, information and technological networks

Social networks are used to represent the interactions among individuals/entities, under a wide range of settings. The study of social networks has its roots in the field of sociology and constitutes a prominent research area for decades (see e.g., Ref. [124]). More recently, the advances in communication and information technologies along with the widespread penetration of the Internet and the World Wide Web (WWW), have led to the explosion of available social networking data. Characteristic examples are the online social networking applications, such as Facebook ([www.facebook.com](http://www.facebook.com)), Twitter ([twitter.com](http://twitter.com)) and Google+ ([plus.google.com](http://plus.google.com)). Of similar importance are several information and technological networks that are part of our everyday life, including the Internet, the World Wide Web network (the hyperlink structure between webpages), and mobile phone communication networks. In many cases, the relationships between entities on such networks are not reciprocal, forming directed edges. Cluster analysis in social, information and technological networks has been proved to be a useful task that can be used to shed light on the structure of these complex systems.

Wang and Wong [101] applied a graph clustering approach based on stochastic blockmodels for directed networks, in order to analyze the strength of ties between students from different socioeconomic backgrounds. According to their study, a set of 27 students (13 male and 14 female) from a single classroom were asked to indicate liking for the other students using one of the following facial expressions: (a) big smile, (b) moderate smile and (c) no smile. The case of big smile indicates an increased liking among students and this information is represented as a directed edge in the network. A more extended study of a directed friendship network of high school students (US National Longitudinal Study of Adolescent Health) has been performed in Refs. [94,56]. Fig. 16 presents the clustering results on this dataset, produced by the method of Newman and Leicht [94].

Similar cluster detection studies have been performed for several other social networks of largest scale, that typically arise in the context of social networking applications. For example, the authors of Refs. [107,106,108] performed cluster analysis in large scale directed social networks with thousands of nodes and edges, such as Slashdot ([slashdot.org](http://slashdot.org)), Epinions ([www.epinions.com](http://www.epinions.com)), Twitter and e-mail exchange networks.

Clustering algorithms can also be applied in the case of directed information networks. The most prominent example here is the World Wide Web (WWW). The nodes of the Web network represent webpages, while the edges hyperlinks between different webpages. Communities in the hyperlink structure of the Web may represent webpages that belong on the same thematic category, and therefore, identifying communities can be helpful in several practical applications such as recommender systems (e.g., Ref. [82]). In a similar way, other hyperlink structures that correspond to directed information networks can be benefited by clustering methods. For example, the well-known electronic encyclopedia of Wikipedia (<http://www.wikipedia.org/>) can be naturally represented as a directed network, where each node corresponds to a lemma and the edges to hyperlinks between different lemmas. Applying clustering methods to the directed network of Wikipedia, one can identify meaningful categories of lemmas [54].



**Fig. 16.** A directed social network representing friendship connections between high school students. The shadowed regions represent the two clusters extracted by the algorithm of Newman and Leicht [94]. The vertex shapes show the ethnicity of the students.

Source: The figure is courtesy of Newman and Leicht [94].

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Another important application on information networks concerns the case of citation networks, i.e., directed networks where the nodes represent documents and the edges capture citation relationships (see e.g., Refs. [1,125]). Clustering methods have been applied in the past to citation networks, in order to understand the connection patterns between scientific papers and more generally, to comprehend the connections between different scientific disciplines. Rosvall and Bergstrom [18] applied their flow-based graph clustering method (see Section 4.4.1) to a citation network of scientific journal papers, creating a map of scientific disciplines as shown in Fig. 17. The general observation is that the structure of sciences can be represented as the letter **U**, with the social sciences on the one side, engineering on the other, joined by medicine, molecular biology, chemistry and physics. Chen and Redner [126] studied the community structure of the citation network of the Physical Review journals family between 1893 and 2007 using modularity optimization techniques, observing interesting properties. Similarly, the authors of Ref. [127] applied community detection methods to a patent citation network, in order to understand the patterns of knowledge transfer between technology fields.

Clustering algorithms have been also applied to partition software systems into smaller units. A software system can be represented by a call graph, i.e., a directed network in which nodes represent the programs of the system and the edges depict calls from one program to another. For example, Bisseling et al. [128] applied graph clustering to partition Java and Cobol programs into smaller modules.

## 7.2. Biological networks

A large number of biological systems can be represented as directed networks. Such an example is the network of metabolic pathways, i.e., series of chemical reactions occurring within a cell. These reactions are connected by their intermediates: the products of the one reaction are the substrates for subsequent reactions.<sup>13</sup> Moreover, metabolic pathways are usually considered in one direction. Numerous distinct pathways co-exist within a cell, forming the so-called metabolic network. A major challenge in biology is to understand the structure and evolution of these networks [129] and graph clustering approaches have been applied towards this goal [130].

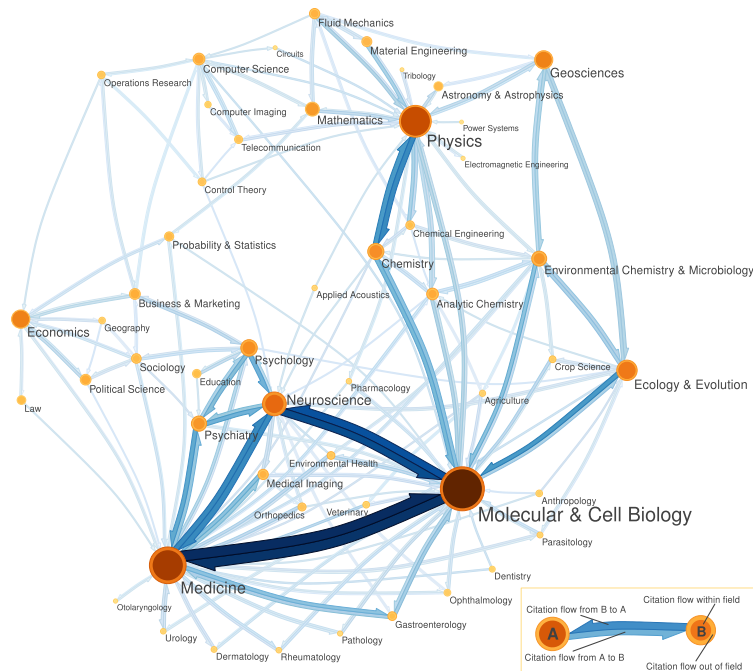
Another important type of biological directed networks are the gene regulatory networks (GRNs). GRNs show the regulatory relationships among genes in a cellular system and are involved in the production of proteins. Broadly speaking, the nodes of a GRN are proteins, mRNAs and protein–protein complexes, while the edges represent individual reactions (protein–protein and protein–mRNA interactions).<sup>14</sup> Clustering tools can be applied to reveal the structural properties of these networks, since densely connected groups may have an important biological interpretation (e.g., Ref. [131]).

In the context of lateral gene transfer and prokaryote genome sequence data, the donor–recipient relations between genomes are modeled by directed networks called Lateral Gene Transfer networks (LGT). Applying graph clustering methods on these networks, we are able to test hypotheses regarding LGT patterns and mechanisms operating in nature [12].

The list of applications in the biological domain continues with the case of food web networks [132,1], which represent trophic relationships in ecosystems. Typically, the nodes of the network correspond to species of an ecosystem and the

<sup>13</sup> Wikipedia's lemma for *Metabolic pathway*: [http://en.wikipedia.org/wiki/Metabolic\\_pathway](http://en.wikipedia.org/wiki/Metabolic_pathway).

<sup>14</sup> Wikipedia's lemma for *Gene regulatory network*: [http://en.wikipedia.org/wiki/Gene\\_regulatory\\_network](http://en.wikipedia.org/wiki/Gene_regulatory_network).



**Fig. 17.** A map of scientific disciplines based on citation patterns of about 6.5 million citations.

Source: The figure is courtesy of Rosvall and Bergstrom [18].

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directed edges capture prey–predator relationships. Regarding the community structure of food webs, the basic question is whether the networks are organized into compartments (the term used to describe the communities–clusters in food webs), where species within the same compartment interact frequently among each other, but show fewer interactions between species of different compartments (see e.g., Refs. [133–135]). The existence of community structure in food webs is an important property, due to its relationship to the robustness of the network under perturbations.

### 7.3. Neuroscience

Neuroscience is the scientific discipline that studies the nervous system and the brain.<sup>15</sup> With the advances in brain mapping and neuroimaging techniques<sup>16</sup> (i.e., techniques used to image the structure and function of the brain), the brain can be modeled by graph structures known as complex brain networks. In recent years, there has been several studies concerning graph theoretical analysis of human brain networks for a wide range of mapping techniques, such as MRI, fMRI and EEG/MEG (see the following review articles in the area [136,137]). Depending on the mapping approach, the nodes of the networks can be defined as the electroencephalography electrodes or multielectrode-array electrodes, or as specific anatomically defined regions of the brain (e.g., regions of MRI or diffusion tensor imaging data). Then, a measure of association between nodes should be selected. Some examples are the measures of spectral coherence or Granger causality between two MEG sensors or the connection probability between two regions of diffusion tensor imaging data. Finally, the adjacency matrix of the graph is typically formed by the pairwise association between nodes (see Ref. [136] for more details). In many cases, the association is not symmetric, forming directed brain networks.

Cluster analysis in human brain networks is an important task, which can help neuroscientists to extract functional subdivisions of the brain. Thus, in the case of directed brain networks, the clustering methods presented throughout this survey paper can be proved useful in the field of neuroscience. Liao et al. [138] studied the directed influence brain network of resting-state fMRI recordings. Among other things, they observed that the network has a modular structure, applying the modularity maximization technique of Leicht and Newman (see Section 4.3.1 and Ref. [50]). The authors also discuss some specific properties that are shared among nodes of the same module. In Ref. [13], the authors examined the directed networks of spontaneous activity correlation or Resting State Networks (RSN), i.e., brain networks that capture spontaneous activity (not stimulus or task driven), applying also the directed version of modularity [50]. Vertes and Duke [139] studied a mechanism of neuronal encoding, investigating the effects of network topology based on spatiotemporal patterns of

<sup>15</sup> Wikipedia's lemma for Neuroscience: <http://en.wikipedia.org/wiki/Neuroscience>.

<sup>16</sup> Wikipedia's lemma for Neuroimaging: <http://en.wikipedia.org/wiki/Neuroimaging>.

spikes. The produced network of neurons is directed and the authors, among other things, applied clustering methods on the analysis. In Ref. [140], directed cortex networks were analyzed, focusing on structural properties such as node betweenness centrality, average shortest path length and community structure. As a last application example from the area of neuroscience, we refer to the work of Pan et al. [141], who studied the nervous system of the nematode *Caenorhabditis elegans*, focusing on its organization into modules.

#### 7.4. Other applications

Directed graph data arises in several other application domains, broadening the scope of clustering methods presented throughout this paper. In the case of financial networks, the authors of Ref. [142] analyzed the community structure of an Italian corporate ownership network, where nodes represent firms (companies), while a directed edge between two firms  $i, j$  captures stock ownership relationship (between the shareholder  $i$  and the owned company  $j$ ). The authors applied modularity maximization techniques [50] on the connected part of this directed network (consisting of 141 nodes), observing strong community structure.

Clustering methods in directed networks can also be used in the field of computer vision and image processing, and more precisely in the task of image segmentation. An image can be modeled as a graph, where pixels are represented as nodes in the graph, and edges capture similarity between different pixels (as computed by a pairwise similarity function on a set of image attributes such as color and intensity). The similarity (or affinity) measure can be either symmetric or asymmetric. In the case of asymmetric affinity measures, the produced graph is directed. Since the initial image has been transformed into a graph, the image segmentation task becomes a graph clustering problem and several new clustering approaches have been proposed for this grouping problem with asymmetric affinities (e.g., Refs. [77,110]).

The range of applications for the clustering problem in directed networks can become very broad, since a large number of non-graph data can be represented as directed graphs using appropriate transformation techniques. Given a set of data points  $x_1, x_2, \dots, x_n$ , where each  $x_i \in \mathbb{R}^N$ , and a similarity measure  $s_{ij} \geq 0$  for all pairs of points  $(x_i, x_j)$ , the data can be represented by a similarity graph  $G = (V, E)$ . In this graph, each node  $v_i \in V$  represents a data point  $x_i$ , while two nodes  $v_i, v_j$  are connected via edge if the similarity  $s_{ij}$  between data points  $x_i$  and  $x_j$  is larger than a specific threshold (the edge can be weighted by the term  $s_{ij}$ ). Then, the data clustering problem can be considered as a graph clustering task; the goal is to partition the similarity graph in such a way that edges across different clusters should have low weight, while high weight edges should be placed within the same cluster. Depending on the method applied to construct the similarity graph, the latter can be either directed or undirected [14]. For example, in the approach of  $k$ -nearest neighbor graph, node  $v_i$  is connected to  $v_j$  if  $v_j$  is among the  $k$ -nearest neighbors of  $v_i$ . This forms a directed graph, since the neighborhood relationship is not symmetric. Hence, in the general case on nonsymmetric similarity functions, i.e.,  $s_{ij} \neq s_{ji}$ , the corresponding similarity graph can be directed.

## 8. Open problems and future research directions

In this section we discuss interesting open problems and future research directions for the graph clustering and community detection task in directed networks. Most of the topics that will be presented shortly also suit to the undirected case of the problem (e.g., see Ref. [11]). However, it seems that the graph clustering problem in directed networks is more challenging compared to the undirected version. Moreover, since the directed case is a generalization of the undirected one (each undirected graph can be also represented as a directed, considering edges to both directions), effective methods for the former case can be used for the latter one as well.

#### Formal definition of the problem

The major point that should be addressed in the area is a formal and precise definition of the graph clustering and community detection problem in directed networks. We have observed that most of the proposed methods follow two high-level clustering notions—definitions (or a combination of them), as described in Section 3. The most prevalent one, the density-based clustering notion, can be considered as a direct generalization from the undirected case, and according to this viewpoint some well-known approaches have been proposed. Although in many of these methods (e.g., modularity optimization) the direction of the edges is taken into consideration in the clustering task, there is no a clear way of how this can be properly done. For example, in the directed version of modularity (e.g., Refs. [50,58]), the existence of a directed edge  $(i, j)$  between nodes  $i, j$ , depends on the out-degree of node  $i$  and in-degree of node  $j$ . Then, the configuration (null) model is suitably adjusted to meet this fact. However, in many cases, different approaches set up diverse requirements for the problem and therefore, many of the proposed methods are not consistent with each other (this has been pointed out for the undirected graph clustering problem as well [11,19]).

As we mentioned in Section 1 regarding the challenges posed by the problem, even some direct generalizations from the undirected graph clustering problem are not straightforward. We have discussed that graph concepts applied to characterize and evaluate the community structure in undirected networks (e.g., density) cannot be directly extended to the directed case, making the theoretical foundations of the problem not yet fully explored. To conclude, we consider that the foremost task

regarding the problem is to establish the theoretical tools towards a formal definition of how good clusters or communities in directed networks should look like. Of course, one should not expect that a single definition would fit to all needs, since as noted by Schaeffer [19], the problem is highly application-oriented (this fact holds for both directed and undirected networks; an evidence for the former case is the plethora of diverse applications presented in Section 7). Later at this section, we will discuss possible data-driven and application-driven methods, as an interesting future direction.

### *Algorithm design and evaluation*

Several interesting points typically arise in the context of designing and evaluating algorithms for the clustering problem in directed networks. Having defined the basic functionalities of the algorithm as well as the type-notion of clusters that we are looking for, three other aspects are of particular significance:

- (a) *Algorithm's parameters*: issues related to the parameters of the algorithm, such as their number, how the user is going to set input values for the parameters, as well as the sensitivity of the algorithm on the parameters' selection.
- (b) *Algorithm's scalability*: issues related to the ability of the algorithm to perform well, while the size of the input (i.e., the size of the graph in our case) increases.
- (c) *Algorithm's evaluation*: issues related to the evaluation of the algorithm, both in terms of computational efficiency and effectiveness.

Any graph clustering algorithm should contain as few parameters as possible, with the ideal case to be the design of parameter-free algorithms. As has been noted in several research articles, this point is extremely crucial while designing data mining algorithms (e.g., see Ref. [143]) for several reasons. First of all, a non-expert user should be able to use the algorithm without any technical difficulties related to the selection of appropriate values for the parameters. Moreover, in the clustering task, incorrect selection of the parameters may lead the algorithm to extract incorrect patterns from the data. Finally, the output of the algorithm (the extracted clusters/communities) should not be highly sensitive to the settings of parameters' values. Some of the community detection algorithms presented in this paper do not require any input parameters (e.g., the methods based on modularity optimization), while others require to select the number of clusters.

The scalability is always considered as an important performance issue in the design and evaluation of graph clustering algorithms, and over the last years it has received great attention from the research community due to the enormous available graph data. Usually, the objective measures used to identify the clustering structure, lead to computational difficult problems; then, either approximation techniques or other novel approaches (or heuristics) are applied to cope with the computational complexity constraints. For example, in the case of undirected networks, Satuluri and Parthasarathy [144] presented a clustering technique based on stochastic flows, that improves in terms of scalability, the well-known Markov Clustering algorithm (MCL) proposed by van Dongen [145] (the authors also note that their method can be easily extended to directed networks). Recently, distributed computing techniques based on the MapReduce framework [112] have become the standard approaches for processing massive data. Several methods have been proposed for analyzing graph data in this framework (e.g., the *Pegasus* system [146]), including spectral graph analysis [147] and centrality estimation [148]. To this direction, it would be interesting to extend already developed algorithms for the clustering problem in directed networks or to design new ones in the MapReduce framework, letting us to study the community structure of very large networks (e.g., billion-node networks).

One other significant point related to the clustering problem in directed networks has to do with the evaluation of methods, i.e., how to decide if the results of an algorithm are "good" or which of several possible clustering results is the best one. As we discussed in Section 6, in case of datasets with a priori knowledge of the community structure, this information can be used to evaluate the performance of the algorithm. However, ground truth data is not always available; then, the goal is to define reliable benchmark graphs that can be used to test and evaluate algorithms. The work of Lancichinetti and Fortunato [123] presents such a generator for benchmark directed networks but we consider that more effort should be put on this topic by the research community due to its importance.

Furthermore, in order to become more clear which clustering algorithm may be better or at least has better performance on specific directed networks, experimental and comparative studies should be done. In the case of undirected networks, several experimental comparisons have been performed for different scale and different types of networks (e.g., social networks, information networks. See Ref. [39,21,23] for more details). We consider that similar studies in directed networks will shed more light on how to select a clustering algorithm.

### *Towards data-driven and application-driven approaches*

It becomes clear that the problem of clustering in directed networks is very challenging and several diverse methods have been proposed to deal with it. We consider that the problem is from its nature application-oriented and thus, there should always be space for new possible solutions depending on the characteristics of the network data and the application domain.

A possible direction is the design of data-driven algorithms for the clustering task in directed networks. According to this approach, the goal is to study the structure of the networks we are interested in, and then take into account possible structural observations that may affect the community detection task; even better would be to exploit possible patterns or



interesting structures that may be contained in the data, in the design phase of an algorithm. Such studies and approaches have already been performed in the case of undirected networks. Some of them study the quality of communities in real networks. Leskovec et al. [149,150] observed that in large scale social and information networks, “good” communities exist only at very small scales (of about 100 nodes), while at larger scales the communities gradually blend in with the rest of the network. Similar observations have been presented by Malliaros et al. [151], studying the robustness of large social graphs. Another example is the community detection algorithm presented by Prakash et al. [152], which exploits the *eigenspokes* pattern observed in large scale sparse real graphs (i.e., pattern related to the eigenvectors of the adjacency matrix of the graph). Thus, it would be useful to perform exploratory analysis regarding the structural properties of directed networks and utilize possible interesting findings to the algorithm design process.

A different possible direction is to follow application-driven approaches, i.e., design domain-specific and application-specific clustering algorithms for directed networks. As we have already mentioned, the graph clustering task can be applied in a wide range of applications, from social network analysis to biological networks and from economic networks to the domain of neuroscience. All these diverse applications demonstrate different features and therefore it should be more appropriate to follow different methodological approaches with respect to the application under consideration.

### Other research directions

In this section we present other, diverse interesting topics for future research regarding the clustering/community detection problem in directed networks (generally, most of the research directions in the case of undirected networks (e.g., Refs. [11,19]) can also be considered as important aspects for directed networks).

A possible direction is to examine local (versus global) definitions of clusters in directed networks and therefore local algorithms for detecting the community structure. In other words, instead of partitioning the full graph, it would be interesting to define measures and design algorithms for evaluating a subgraph in terms of community structure. Such approaches can also operate as *community structure exploration* tools and may be useful either for large scale networks or for networks with no clear community structure (e.g., Ref. [150]).

Generally, in the discussion until now, the directed networks represent mainly connectivity information between entities of the same type; the edges may or may not contain weights, which quantify the significance of the ties and typically are interpreted as deterministic values with positive meaning. However, new domains and applications in the context of network analysis, impose new kind of information that should be also taken into consideration in the clustering task. Three well known representative examples are the so-called signed networks, probabilistic (or uncertain) networks and the case of heterogeneous networks. The *signed networks* (e.g., Refs. [153,154]) are trying to capture the notion of positive and negative interactions among the nodes of a network. A positive edge denotes similarity (proximity), while negative edges represent dissimilarity (distance). Signed networks can be both directed and undirected. Characteristic examples of directed signed networks are the trust networks between users in product review websites, like Epinions ([www.epinions.com](http://www.epinions.com)). The *probabilistic graphs* (e.g., Refs. [155–157]) capture uncertainty that is introduced under several conditions (such as for privacy-preserving reasons), and every edge in the network is associated with its probability of existence. Since probabilistic graphs is the natural extension of deterministic ones to represent uncertainty factors, they can be both directed and undirected. For the undirected case, Kollios et al. [157] recently presented an algorithm for the graph clustering task. Finally, *heterogeneous networks* (in contrast to homogeneous ones) [158], directed or undirected, are used to represent multi-typed networks, i.e., networks that contain multiple objects and link types (e.g., in a bibliographic network the nodes may correspond to authors, publications and venues, while the edges link these different types of nodes). An interesting research question is how can we extend existing techniques or design new ones for the clustering task in directed networks under the settings presented above.

Finally, an important research direction which has been already discussed, is the case of dynamic directed networks, i.e., networks that evolve over time with the addition/deletion of nodes/edges. In Section 4.4.4 we described a method for time-evolving directed networks, where the goal was both the extraction of the community structure and the detection of a change point (regarding community structure) over time.

## 9. Conclusions

In this survey we have reviewed thoroughly the problem of clustering and community detection in directed networks and to the best of our knowledge, this is the first comprehensive review fully devoted to the problem. The main goal was to organize and present in a unified manner the work conducted so far for the problem. In a first step, we have presented a classification of the approaches in four main categories, according to the methodology they follow: (i) naive graph transformation approaches, (ii) transformations maintaining directionality, (iii) approaches that extend objective functions and methodologies to directed networks, and (iv) alternative approaches. Since a large portion of the methods constitute extensions from the undirected version of the problem, we have followed an incremental presentation, describing the basic features of the undirected problem and how they can be extended to the directed case. Furthermore, we have presented a second orthogonal classification of the methods, based on the clustering notion (or type of clusters) they follow. This classification scheme is supplementary to the previous one and it may be useful for practitioners that need to select an appropriate algorithm for a specific application. We have also presented methods and tools for evaluating and testing

the results of a graph clustering algorithm in directed networks. Moreover, since the problem is highly application oriented, we have demonstrated interesting application domains. To conclude, we consider that more effort should be put on the problem by the research community due to its high importance, and towards this direction we have provided interesting topics for future research.

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