Comparison and validation of community structures in complex networks

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Abstract

The issue of partitioning a network into communities has attracted a great deal of attention recently. Most authors seem to equate this issue with the one of finding the maximum value of the modularity, as defined by Newman. Since the problem formulated this way is NP-hard, most effort has gone into the construction of search algorithms, and less to the question of other measures of community structures, similarities between various partitionings and the validation with respect to external information.

Here we concentrate on a class of computer generated networks and on three well-studied real networks which constitute a bench-mark for network studies; the karate club, the US college football teams and a gene network of yeast. We utilize some standard ways of clustering data (originally not designed for finding community structures in networks) and show that these classical methods sometimes outperform the newer ones. We discuss various measures of the strength of the modular structure, and show by examples features and drawbacks. Further, we compare different partitions by applying some graph-theoretic concepts of distance, which indicate that one of the quality measures of the degree of modularity corresponds quite well with the distance from the true partition. Finally, we introduce a way to validate the partitionings with respect to external data when the nodes are classified but the network structure is unknown. This is here possible since we know everything of the computer generated networks, as well as the historical answer to how the karate club and the football teams are partitioned in reality. The partitioning of the gene network is validated by use of the Gene Ontology database, where we show that a community in general corresponds to a biological process.

Key words: network, community, validation, distance measure, hierarchical clustering, K-means, GO
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1 Introduction

Complex networks, i.e., assemblies of nodes and edges with nontrivial properties, can be used to describe systems in many different fields, such as sociological (scientific collaborations and structure of organizations, biological (proteins and genes interactions and technological (Internet and the web). These systems are composed of a large number of interacting agents, and the complexity originate partly from the heterogeneity in their interaction patterns. Given this high degree of complexity, it is often necessary to divide a network into different subgroups to facilitate the understanding of the relationship among different components [8,31,23]. Outlines of recent work are given in, e.g., [6,4] together with broad discussions of relevant literature.

In recent years there has been an increasing interest in the properties of networks, and the property of community structure has attracted great attention. The vertices in the networks are often found to cluster into tightly-knit groups with a high density of within-group edges and a lower density of between-group edges. Clustering techniques have acquired a dominant role among the tools used to decompose the network into functional units. Community structure is a topological property of networks and it is linked to the concept of classification of objects in categories. The working definition of community is general, but ambiguous. There is no generally accepted formal definition, but an informal one is “a subset of nodes within the graph such that connections between the nodes are denser than connections with the rest of the network”, see Fig.1. That is, a community can be seen, depending on the context, as a class, group, cluster etc. Communities in a social network might represent real social groupings, perhaps by interest or background; communities in a citation network might represent related persons on a single topic, communities in a gene networks might represent specific biological processes, communities on the web might represent pages on related topics, and so on. Being able to identify these communities could help us to understand and exploit these networks more efficiently.

![Fig. 1. Example of a small network with community structure.](image-url)
Since the issue of community detection has acquired relevance in several fields, a great interest has raised on the algorithms used to determine communities in a network. Several algorithms to determine communities are known in the literature. A survey of the different approaches can be found in [21,20], and especially in [4] where these approaches are evaluated with respect to computational cost and sensitivity. In the present paper, we return to two classical methods of finding groups among data—the hierarchical clustering and the K-means. Both of these methods are well-known within the applied statistics community [26], but at least the former has in some papers been discarded as a less suitable way of finding communities in a network [8,20]. One of our results is that this rejection was a bit premature—with a suitable metric for the distances between the nodes, the result of such a hierarchical clustering can outperform some of the more modern approaches. The K-means has not, to the best of our knowledge, been utilized before for finding community structures in complex networks.

The present paper focuses on networks with a single type of vertex and a single type of undirected, unweighted edges. As examples, we consider simulated networks (originally described in [8]) and three real examples from the literature—Zachary’s karate club [30], the college football teams in US division one for the year 2000 [8] and a gene network of the yeast *Saccharomyces cervisiae* [17]. By using different quality measures, we explore how well the two methods we study perform, and by using distance measures for partitions we also investigate how similar the communities found by different algorithms are. Finally, we introduce an external validation method which works also for only partially known networks. The article is written to be as self-contained as possible, which means that we introduce rather carefully also concepts that are well described elsewhere in the literature. However, several of the sources are scattered among different scientific areas, and therefore we consider it as meaningful to repeat them here. Careful references are always given, though, when the concepts are not new.

The idea of the disposition of this article is to carefully introduce new concepts in almost direct relation to the networks to which they are applied for the first time. This takes the following form:

- **Section 2** introduces the tools we utilize for finding community structures in the networks, particularly
  - metrics for distances between the nodes.
  - clustering algorithms (hierarchical clustering and K-means).
- **Section 3**, the karate club network, with the concepts
  - modularity.
  - Silhouette index.
  - a null hypothesis by rewiring.
  - measures and indices of the similarity of two partitionings.
- **Section 4**, computer generated networks, with illustrations of most of the concepts introduced thus far.
Section 5, US college football teams, with
- a novel coherence score, measuring how well the detected modules correspond
to an external classification of the units of the network.

Section 6, a gene network from yeast. This time, no “true” partitioning exists,
and we apply the different methods introduced earlier in this article in order to
see whether we can obtain a biological meaningful division of the network.

Section 7, a general discussion of the results obtained and conclusion of the paper

2 Detecting community structures

This section introduces the algorithms we utilize for detecting communities. It com-
prises several ideas scattered through the literature, and its purpose is to make the
article self-contained. However, the reader is still referred to the references for more
detailed descriptions of the central concepts.

2.1 Distance between nodes

First we need a way to measure distance between nodes in the networks. The most
common way is to consider the geodesic, that is, the shortest path (counted in num-
ber of links) connecting two vertices. The geodesic distance between two nodes is
then just the minimum number of links which separate them. For future reference
we denote the matrix of all pairwise geodetic distances as $G$.

In [8] Girvan and Newman propose to define the distance between vertices as the to-
tal number of paths that run between them. However, the number of paths between
any two vertices is infinite (unless it is zero) so paths of length $\ell$ are weighted with
a factor $\alpha^\ell$ with $\alpha$ small, so that the weighted count of the number of paths con-
verges. In this way, long paths contribute with less weight than those that are short.
If $A$ is the adjacency matrix of the network, such that $A_{ij}$ is unity if there is an edge
between vertices $i$ and $j$ and zero otherwise, then the distances are given by the
elements of the matrix $W$, calculated as

$$W = \sum_{\ell=0}^{\infty} (\alpha A)^\ell = (I - \alpha A)^{-1}. \quad (1)$$

For the sum to converge, $\alpha$ must be chosen smaller than the reciprocal of the largest
eigenvalue of $A$. Both these definitions of distances give reasonable results for com-
munity structures, but in some cases they are less successful. Different authors have
used different approaches for the choice of the weights but it has not, to the best
knowledge of the present authors, been made a systematic comparison between
clustering algorithms implemented with different choices of distances.
Both measures result in a matrix \((G\text{ or } W)\) of dimension \(n \times n\) (where \(n\) denotes the number of nodes in the network) whose elements are the distance between the nodes in the network.

Eventually, we utilize as distance measure between node \(i\) and \(j\) the euclidean distance between the \(i\)th and \(j\)th row in one of the matrices \((G\text{ or } W)\) above. That is, we take

\[
dist(\text{node } i, \text{node } j) = \sqrt{\sum_{k} (P_{ik} - P_{jk})^2}, \quad (2)
\]

where \(P = G\) for the geodesic distance and \(P = W\) for the sum of all paths. This way, the issue of finding communities in a network becomes algorithmically identical to finding clusters from co-variation within a series of experiment, and standard routines available in, e.g., MatLab, R, etc. can be used. A similar approach with respect to (2) and hierarchical clustering, but with a different \(P\), has been suggested in [24] and applied to a protein-protein interactions network.

### 2.2 Community detecting algorithms

The following two standard algorithms have been implemented and tested:

- Hierarchical clustering.
- K-means algorithm.

Of course, our choice of tested algorithms is not intended to be exhaustive, but we have focused on some algorithms that are well-known clustering methods, but have not been applied systematically to complex networks.

Hierarchical clustering [7] is an unsupervised procedure of transforming a distance matrix, which is a result of pair-wise similarity measurement between elements of a group, into a hierarchy of nested partitions. It is an agglomerative procedure, which means that it starts with as many clusters as there are nodes, i.e., each node forms a cluster containing only itself. Iteratively the number of clusters is reduced by a merging of the two most similar clusters until only one cluster remains. Once several nodes have been linked together, a linkage rule is needed to determine if two clusters are sufficiently similar to be linked together. Different linkage rules have been proposed. In this paper complete linkage, also called furthest neighbour is used. This method utilizes the largest distance between nodes in two groups. Explicitly, it takes the form

\[
d(r, s) = \max_{i,j} \left( \text{dist}(x_{ri}, x_{sj}) \right), \quad i = 1, \cdots, n_r, \quad j = 1, \cdots, n_s \quad (3)
\]
where \( n_r \) and \( n_s \) are the numbers of nodes in clusters \( r \) and \( s \), respectively, and \( x_{ri} \) denotes the \( i \)th node in cluster \( r \).

K-means [11] is a clustering algorithm that is widely used when working with temporal data where the elements should be grouped on the basis of their time profile. Data are clustered into \( N \) mutually exclusive clusters, where \( N \) has to be chosen beforehand. It uses an iterative algorithm that minimises the sum of distances from each object to its cluster centroid, over all clusters. The algorithm moves the objects in a deterministic fashion between the clusters until the sum cannot be decreased further. The result is a set of clusters that is as compact and well-separated as possible, given the initial partitioning. A drawback of the K-means algorithm is that it often converges to a local optimum. This problem can be somewhat remedied by choosing multiple starting points. For what we are aware of there have not yet been systematic studies of the use of K-means algorithm to detect community structure in networks.

3 Zachary’s karate club

Zachary observed 34 members of a karate club over a period of 2 years. During the course of the study, a disagreement developed between the administrator of the club and the club’s instructor, which ultimately resulted in the instructor leaving and starting a new club taking about half of the original club’s members with him.

Zachary constructed a network of friendship between members of the club, using a variety of measures to estimate the strength of ties between individuals. Here we use a simple unweighted version of his network with the attempt to identify the factions involved in the split of the club (see [8], [30]). The network\(^1\) consists of 34 nodes and 78 links as illustrated in Fig. 2; squares denote the supporters of the trainer (node 1) and circles represent the supporters of the administrator (node 34).

When we apply the community detecting algorithms described in Sec. 2 above, we also need a way of deciding upon the number of communities we should have. One way of getting this number, when we do not have prior knowledge, is to measure the quality of the partitioning itself and simply pick the number which results in the “best” clustering. However, in accordance with the ambiguity mentioned in the introduction about what is meant by community structure, there exist several different measures for the quality of the partitioning of a set of nodes into communities. Here we will discuss two such measures, the Silhouette index [2] and the modularity [8].

\(^1\) The network can be downloaded from [http://vlado.fmf.uni-lj.si/pub/networks/data/UciNet/UciData.htm](http://vlado.fmf.uni-lj.si/pub/networks/data/UciNet/UciData.htm) and the graphical representation of the network is obtained from [http://www-personal.umich.edu/~mejn/networks/](http://www-personal.umich.edu/~mejn/networks/); see [8].
3.1 Evaluation of the strength of the community structure, modularity

The first measure we consider is Newman’s modularity [19], which has become a kind of de facto standard for measuring the quality of a partitioning (although there are alternatives coming, e.g., [18,15]).

The modularity is defined the following way: Given a particular division of a network into $k$ communities, let $e$ denote a $k \times k$ matrix whose element $e_{ij}$ is the fraction of all edges in the network which connect vertices in community $i$ to those in community $j$. The trace of this matrix $\mathrm{Tr} e = \sum_i e_{ii}$ gives the fraction of edges in the network that connect vertices in the same community. A good community division should have a high value of the trace, but the trace on its own is not a good indicator of the quality of the division since, for example, placing all vertices in a single community would give the maximal value of $\mathrm{Tr} e = 1$ without giving any information about the community structure. The row (column) sum is then defined as $a_i = \sum_j e_{ij}$ and it represents the fraction of edges that connect to vertices in community $i$. In a network where edges fall between vertices without regard for the communities they belong to, it holds $e_{ij} = a_i a_j$. The modularity is therefore defined as

$$Q = \sum_i \left( e_{ii} - a_i^2 \right).$$

(4)

It measures the fraction of edges in a community, minus the expected value of the same quantity in a network with the same community divisions but random connections between the nodes. If a particular division gives no more within-community edges that would be expected by random chance the modularity is zero. Values other than 0 indicate deviations from randomness, and as a rule of thumb, values above 0.3 indicate a modular structure [22]. In practice, values above 0.7 are rare, and indicate a very clear structure. However, also Erdős-Rényi (ER) random graphs can possess a very high modularity, as shown in [9]. The reason is that there are so many different ways to partition a network, that it is likely that there should be at least one partition where the intra-density of links within a cluster greatly exceeds the one obtained by chance. Because of this, we consider below in Section 3.3 a null hypothesis where the networks are rewired.
We apply the K-means and the hierarchical clustering methods to the Karate club, both when the distances are the geodetics and when they are a sum over all paths. By calculating the modularity for every possible number of partitions, from one up to 34, we can easily see what the “best” division is. For each partition the modularity $Q$ is computed and is plotted in Fig. 3 (for the K-means, we took the division among the repetitions with the same number of communities resulting in the highest $Q$, and discarded the rest). We can immediately see that the hierarchical algorithm

![Fig. 3. Modularity $Q$ for the communities detected in Zachary’s karate club. Solid curve: hierarchical clustering (shortest path), dashed curve: K-means clustering (sum of paths), dotted curve: K-means clustering (shortest path), dash-dotted curve: hierarchical clustering (sum of paths).](image)

applied with the distance given by the sum of all the paths (1) gives always negative values of $Q$; this means that the partitions obtained do not correspond to communities of the network. The other algorithms, instead, can all partition the network into communities. For each algorithm we have analysed the partition corresponding to the highest modularity $Q$, and the results are presented in Table 1.\(^2\)

The K-means algorithm used with the sum of paths distance between nodes detects two communities and all the nodes are partitioned according to the sociological division that took place in the club (circles and squares of Fig. 2 are divided into two separate groups). When both the K-means algorithm and hierarchical cluster-

\(^2\) We note that our peak value, $Q = 0.4198$, slightly exceeds the maximum we have found in the literature, $Q = 0.4188$, in [5].
Table 1
Karate club: highest modularities obtained using different approaches and their corresponding community structure computed for the true network ($Q$) and for the rewired network representing the null hypothesis ($Q_{H_0}$).

| Algorithm                  | $Q$  | No of clusters | $Q_{H_0}$ | No of clusters |
|----------------------------|------|----------------|-----------|----------------|
| Hierarchical (shortest path) | 0.42 | 4              | 0.22 ± 0.04 | 9              |
| K-means, (sum of paths)    | 0.37 | 2              | 0.15 ± 0.02 | 9              |
| K-means, (shortest path)   | 0.34 | 4              | 0.18 ± 0.07 | 3              |

Looking in details we see that in both cases the 4 communities represent a further division of the 2 factions created in the club. This means that the union of communities 1 and 2 is exactly the group of supporters of the trainer and the union of communities 3 and 4 contains all the supporters of the administrator.

3.2 Evaluation of the strength of the community structure, Silhouette index

The second measure we discuss is the Silhouette index [25,2,3]. This measure is wide-spread in the context of clustering based on co-variation over several experiments, and since we explore such methods here, a discussion of the measure is most appropriate.

For each cluster, one can calculate the Silhouette index, $S_j$, which characterizes the heterogeneity and isolation properties of the cluster. The Global Silhouette index, $GS$, is the mean of all the Silhoutte indices (one for each cluster) for the set, and can be used as an effective validity index.

A drawback of the Silhouette index is that a community consisting of only one node is considered to be a perfect partitioning, i.e., the confidence indicator becomes unity. Thus, this measure will be inclined towards such clusters, which makes it a less suitable candidate for measuring the quality of a partitioning. This effect can be eliminated by modifying the average by discarding all the terms in the sum corresponding to clusters with only one element. This is what has been implemented here.

This index has been computed for all the partitions detected by the hierarchical algorithm with both the shortest path distance and the sum of paths distance between nodes, i.e., for one partitioning which works reasonable and for one which gives nonsensical results for the modularity. The results are shown in Fig. 4. The figure shows that in both cases the Silhouette index has the maximum value for $N = 2$, that is, when the set is divided into two clusters. Checking the corresponding partitions we see that when the hierarchical clustering (shortest path) is used,
the maximum of the Global Silhouette index really corresponds to the real structure of the set. On the other hand the partition corresponding to two communities detected by hierarchical clustering (sum of paths) has one cluster containing only one node (node 34: the administrator) and all the other nodes are grouped together. This partition is clearly quite far from the original one while the Global Silhouette index still has a numerical value that in literature is considered to indicate a community structure.

The Global Silhouette index is obviously less suited for estimating the quality of a network partitioning, and in the sequel of the present paper we will only utilize the modularity for measuring the degree of community structure. Further, since the algorithm based on hierarchical clustering (sum of paths) does not seem to work, we will also exclude that one from all further considerations.

3.3 Rewiring

The results obtained are here tested with respect to the null hypothesis that the found community structure is solely due to the degree distribution. This testing is necessary, since it has been shown that also random networks can possess a high modularity [9]. Each network is rewired according to the algorithm presented in [14]. This algorithm randomly rewires a network while preserving the degrees of each node. In this way, we investigate if the communities detected by the algorithms might have occurred by the degree distribution only, or if they represent an intrinsic structure of the network beyond the most obvious one. The three different clustering schemes (hierarchical clustering (sum of paths) is discarded) are applied to the rewired network and the modularity $Q$ is computed. This procedure is repeated 100 times, and the results are shown in Table 1. For each clustering procedure the mean of the $Q$ value is computed over all the repetitions. The $Q$ value is reported together with the corresponding standard deviation. The values of the modularity obtained for the rewired networks are much smaller with respect to the true network; this
shows that the partition detected in the network have not occurred from the degree distribution only.

### 3.4 Distance between partitions

A less studied property, at least in the recent physics literature on networks, is how to compare two different partitionings of the same network with each other. Different definitions of distance between partitions can be found in the literature (see, e.g., [16] for an early comparison of different measures), and here we discuss two of these. In the next subsection, we will compare these measures with two indices that have recently been advocated within this context. For both measures, we need the concept of meet of two partitionings. Let $A$ and $B$ denote two partitionings of the whole set, with corresponding elements $a_i$, $i = 1, \ldots, |A|$ and $b_i$, $i = 1, \ldots, |B|$, which are sets themselves. The meet is then the set $C$ given by

$$C = \bigcup_{i=1}^{|A|} \bigcup_{j=1}^{|B|} \{a_i \cap b_j\}.$$  

(5)

The two distance measures we discuss here are:

$m_{\text{moved}}$: The distance between the partitioning $A$ and the meet $C$, given the partitioning $B$, is defined as the minimum number of elements that must be moved between the partitions so that $A$ and $C$ become identical [10]. The distance between $A$ and $B$, also denoted as the total distance, is then obtained as the sum of the distance between $A$ and $C$ and the distance between $B$ and $C$. (Alternative, but equivalent, definitions can be found in [10,29].)

$m_{\text{div}}$: The distance between the partitioning $A$ and the meet $C$, given the partitioning $B$, is defined as the minimum number of divisions that must be implemented in $A$ so that $A$ and $C$ become identical [27]. The distance between $A$ and $B$, the total distance, is then obtained in the same way as for $m_{\text{moved}}$, i.e., as the sum of the two partial distances.

These definitions give different results when applied to general partitions. In order to understand how two partitions are related to each other, both measures are useful, as shown by the example below.

**Example 1 (Distances between two partitions)**

Let $n = 9$, and let $A$ and $B$ be the two partitions $A = \{\{1, 2, 3, 4, 5, 6\}, \{7, 8, 9\}\}$ and $B = \{\{1, 2, 4, 5, 7, 8\}, \{3, 6\}, \{9\}\}$. The meet from (5) is then given by $C = \{\{1, 2, 4, 5\}, \{3, 6\}, \{7, 8\}, \{9\}\}$. The measures computed according to the two methods above are shown in Table 2. It shows that the two definitions of distance between partitions may give different measures. The information provided by the two methods is significant, in fact both the information on how many divisions must be performed or how many elements must be moved are relevant in order to find out
the relationship occurring between partitions. The distance from partition A to the meet is 3 according to the first method, $m_{\text{moved}}$, and this means that three elements (elements 3, 6 and 9) must be moved but we don’t know how these three elements are grouped in partition B. This information is given by the measure computed with the second method, $m_{\text{div}}$: only two divisions are necessary and this implies that elements 3, 6 and 9 belong to two different clusters in partition B. When comparing partition B with respect to A, the measure $m_{\text{moved}}$ gives the distance from partition B to the meet equal to two, in fact elements 7 and 8 must be moved in order to obtain two partitions with the same clusters. Furthermore, the measure $m_{\text{div}}$ says that these two elements belong to the same cluster in A and therefore it can be seen as a subcluster. If the distance computed by $m_{\text{div}}$ is much smaller than the distance given by $m_{\text{moved}}$, it means that many subpartitions are present; elements belonging to the same original partitions are grouped together.

Table 2
Distance between partitions A and B of Example 1 where distA (distB) denotes distance from A (B) to the meet and distAB the total distance between partitions.

| Method  | distA | distB | distAB |
|---------|-------|-------|--------|
| $m_{\text{moved}}$ | 3     | 2     | 5      |
| $m_{\text{div}}$   | 2     | 1     | 3      |

For the partitions of Table 1 for the Karate club, the distance from the original division of the set (the one represented in Fig. 2) has been computed using both definitions given above. The results are illustrated in Table 3.

Table 3
Karate club: distance between the partitions with highest $Q (P)$ and the meet, and the original division ($P_0$) and the meet.

| Algorithm                | No of clusters | $m_{\text{moved}}$ | $m_{\text{div}}$ |
|-------------------------|----------------|--------------------|-------------------|
|                         |                | distP   | dist$P_0$ | distP   | dist$P_0$ |
| Hierarchical (shortest path) | 4              | 0       | 11      | 0       | 2         |
| K-means (sum of paths) | 2              | 0       | 0       | 0       | 0         |
| K-means (shortest path) | 4              | 1       | 16      | 1       | 3         |

Table 3 shows that the partition produced by hierarchical clustering (shortest path), $P$, represents a subpartition of the original division, $P_0$; in fact the distance from the obtained partition $P$ to the meet is zero. K-means algorithm (shortest path), instead, misclassifies one element: this can be seen from the fact that the distance $m_{\text{moved}}$ from $P$ to the meet is one meaning that one element must be moved in order to have the partition $P$ equal to the original division. K-means algorithm with distance given by the sum of all paths, clearly, detects a partition that is identical to the original division occurred in the club.
3.5 Similarity between partitions

Two well-established indices for the similarity between two partitionings of a set are the Jaccard index and the mutual information index. They are defined as:

\( I_J(A, B) = \frac{n_{11}}{n_{11} + n_{01} + n_{10}} \)

where \( n_{11} \) denotes the number of pairs of elements that are simultaneously joined together in partition \( A \) and \( B \), \( n_{01} (n_{10}) \) denotes the number of pairs of elements that are joined (separated) in \( A \) and separated (joined) in \( B \). It results in a matching coefficient in a range \([0 \ 1]\) where a value of 1 indicates that the two partitions are identical. The Jaccard index was originally developed to assess similarity among distributions of flora in different geographic areas [12].

\( I_{\text{NMI}} \): The normalized mutual information index is a measure of similarity between partitions \( A \) and \( B \) [13,28]. It is based on the mutual information between the partitions when the two partitions are treated as (nominal) random variables. The normalized mutual information index can be expressed as

\[
I_{\text{NMI}}(A, B) = \frac{-2 \sum_{i=1}^{\|A\|} \sum_{j=1}^{\|B\|} n_{ij}^{ab} \log \left( \frac{n_{ij}^{ab} \cdot n}{n_i \cdot n_j} \right) \cdot \log \left( \frac{n}{n_i} \right)}{\sum_{i=1}^{\|A\|} n_i \log \left( \frac{n_i}{n} \right) \cdot \sum_{j=1}^{\|B\|} n_j \log \left( \frac{n_j}{n} \right)} ,
\]

where \( n_i^a \) represents the number of units in cluster \( a_i \) and \( n_{ij}^{ab} \) denotes the number of shared elements between clusters \( a_i \) and \( b_j \). It can be shown that \( 0 \leq I_{\text{NMI}} \leq 1 \) with \( I_{\text{NMI}}(A, A) = 1 \).

In order to compare these two indices with the two distance measures introduced in the previous section, we turn the measures into indices by

\[
I_{\text{moved}} = 1 - \frac{m_{\text{moved}}}{n} \quad \text{and} \quad I_{\text{div}} = 1 - \frac{m_{\text{div}}}{n} \, ,
\]

where \( n \) is the number of units in the partitioned set. In Fig. 5 we show how these four indices vary for the partitionings obtained by hierarchical clustering (shortest path) for the Karate club, when we compare with the actual division which took place.

The index \( I_{\text{div}} \) is a straight line, which indicates that one more node has been misclassified per extra community which is considered. The other three indices behave somewhat similar, with the exception of the mutual information, \( I_{\text{NMI}} \), which does not tend to zero for the limiting case when all nodes are placed in one cluster each.
As discussed in the previous section, the measures $m_{\text{div}}$ and $m_{\text{moved}}$ can be interpreted as the number of divisions and the number of movements, respectively, which are necessary for making two sets coincide. Further, for $m_{\text{div}}$ and $m_{\text{moved}}$ we obtain also partial measures which directly show if one partition is a subpartition of the other. Because of this direct interpretation, the property of showing subpartitions, and the similarity with the other measures when considered as indices, we stick in the sequel of this paper to $m_{\text{div}}$ and $m_{\text{moved}}$.

4 Computer generated networks

Now we consider a class of computer generated random networks. These networks, originally introduced in [8], consist of 128 nodes each, divided into four communities of equal size. The links are distributed randomly, with the same probability for a link to occur for each pair of intra-community nodes, and another constant probability for each pair of inter-community nodes, such that the average degree of each node becomes 16. Intra-community degrees, i.e., the part of the degree that stems from links within the same community, are denoted as $z_{\text{in}}$, and the inter-community degree as $z_{\text{out}}$.

By applying the algorithms introduced above (100 times) to the networks with $0 \leq z_{\text{out}} \leq 10$, we can compare our methods to some others studied in the literature. In Fig. 6 we show the fraction of correctly classified nodes for our three algorithms for different values of $z_{\text{out}}$. It turns out that the K-means clusterings (both measures) give results which are comparable to methods that are very recently developed in order to take care of this community detection problem [5]. Indeed, the results of the two K-means algorithms are identical, which make these computer generated networks unique among the ones we study. This might reflect that these networks are in some sense less complex than the real-world networks, but this issue deserves
a further investigation before any definitive conclusions can be drawn. The fraction
of nodes that are classified correctly by hierarchical clustering (shortest path) is
lower, but the result still makes sense as 60% of nodes are correctly classified when
\( z_{out} = 8 \).

![Graph](image)

**Fig. 6.** Fraction of correctly classified nodes (upper curves for low \( z_{out} \)) and distances from
the true partition (lower curves for low \( z_{out} \)) for computer generated networks, as measured
by \( m_{\text{div}} \) and \( m_{\text{moved}} \) (\( m_{\text{div}} \leq m_{\text{moved}} \)). **Solid curves:** hierarchical clustering (shortest path),
**Dashed-dotted curves:** K-means clustering (shortest path and sum of paths coincide). Each
point is an average over 100 different networks. Typical values of the modularity, obtained
from the true partition, are marked.

However, to measure only the fraction of correctly classified nodes might give a
wrong picture of performance, as noted also in [4]. For instance, if the community
detecting algorithm happens to divide one correctly identified cluster into two, it
is normally not a serious error, but still the fraction correctly classified nodes will
decrease drastically.

If we instead consider the measure \( m_{\text{div}} \) introduced above, we can see that the
deviation from the real structure is quite modest. In Fig. 6, we also depict the two
distance measures \( m_{\text{moved}} \) and \( m_{\text{div}} \) (total distance), which in some sense give a bet-
ter description of the outcome from the algorithms. Here, however, we clearly see
how these different descriptions give similar results.
5 College football

United States college football is now considered [8]. The network represents the schedule of Division 1 games for the year 2000 season: the 115 vertices in the graph represent teams (identified by their college names) and the 613 edges represent regular-season games between the two teams they connect. The community structure is well-known. Teams, in fact, are divided into 13 conferences containing around 8-12 teams each. Games are more frequent between members of the same conference than between members of different conferences, with teams playing an average of about seven intra-conference games and four inter-conference games in the year 2000 season. Interconference play is not uniformly distributed, teams that are geographically close to one another but belong to different conferences are more likely to play one another than teams separated by large geographic distances.

We have repeated the same clustering procedures as above to this data and the results are reported in Fig. 7 and the most prominent features are emphasized in Tables 4 and 5. All algorithms are able to partition the network into communities. The highest value of the modularity $Q$ for each algorithm has been determined and the result is reported in Table 4 together with the corresponding community structure and the results of the null hypothesis test.

| Algorithm                  | $Q$  | #clusters | $Q_{H_0}$       | #clusters |
|----------------------------|------|-----------|-----------------|-----------|
| Hierarchical (shortest path) | 0.46 | 8         | 0.23 ± 0.010    | 7         |
| K-means (sum of paths)     | 0.60 | 11        | 0.28 ± 0.006    | 5         |
| K-means (shortest path)    | 0.60 | 10        | 0.27 ± 0.007    | 5         |

The K-means algorithm gives similar results in both cases with distance between nodes given by (1) and given by the shortest path between the nodes. Two different partitions are determined with the only difference being that in the latter partition one conference is broken into two pieces and grouped with two other conferences. This is the reason why we in Fig. 7 (a) and (b) only show the results from one of the K-means algorithms and from the hierarchical clustering.

The resulting partition is very close to the real conference structure of the 2000 season. The fact that only 11 partitions are detected is because two of the conferences are identified as one conference (this happens also with the other algorithms).

The modularity for the true division into conferences is $Q = 0.537$, which is smaller than the peak we obtain, $Q = 0.6044$. 

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3 The modularity for the true division into conferences is $Q = 0.537$, which is smaller than the peak we obtain, $Q = 0.6044$. 

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There are 5 independent teams that do not belong to any conference and they tend to be grouped with the teams with which they are most closely associated. There are only three teams that are misclassified.

For the partitions of Table 4 the distance from the original division of the set has been computed using both measures $m_{\text{moved}}$ and $m_{\text{div}}$. The results are illustrated in Table 5 and in Fig. 7 (c) and (d).

Here it is clear that the partition closer to the original set is the one detected by K-means algorithm (sum of paths) as distance between nodes, in fact only 14 elements must be moved in order to make the set coincide with the meet.

Both partitions obtained with K-means algorithm (using both definitions of distance between nodes) correspond to high values of the modularity $Q$ so it can be interesting to see how distant these two partitions are between each other. Let $P_{\text{KW}}$ denote the partition obtained with the K-means algorithm (sum of paths)
Table 5
College football network: distance between the partitions (P) with highest Q and the meet, and between the original division (P₀) and the meet.

| Algorithm                        | No of clusters | m\text{moved} | m\text{div} |
|----------------------------------|----------------|---------------|-------------|
|                                  |                | distP | distP₀ | distP | distP₀ |
| Hierarchical (shortest path)     | 8              | 50    | 24    | 25    | 20    |
| K-means (sum of paths)           | 11             | 14    | 5     | 5     | 3     |
| K-means (shortest path)          | 10             | 21    | 9     | 9     | 6     |

(N = 11), and P_{KG}, the partition obtained with the K-means algorithm (shortest path) (N = 10). The distances to the meet from respective partition become m\text{moved}(P_{KW}, meet) = 6, m\text{moved}(P_{KG}, meet) = 12, m\text{div}(P_{KW}, meet) = 2, and m\text{div}(P_{KG}, meet) = 3. The total number of elements to be moved in the two partitions in order for them to become identical is 18. If 6 elements are moved within the communities of P_{KW}, then P_{KG} becomes a subpartition (as the number of partitions is different). These two partitionings are thus closer to each other than any of them to the “true” partitioning, hence at least in this case the choice of algorithm seems less crucial.

**Coherence score**

If the true partition of the network is not known, we have to turn to another way of validating the structure than to measure the distance. A common case is that we have annotations (one or many) to each node, and that we should utilize in some way the property that some of these annotations are common to more than one node. Here we propose the following method, illustrated by the simplest case where each node has exactly one annotation:

Assume every node in the network has a classification—here it is the conference to which it belongs. To judge the quality of a specific community partitioning, let us take one of the modules we detected as an example. This module contains in total ten teams, with eight teams from one conference and two teams from another conference. Given the actual sizes of these two conferences, the total number of teams and the total size of this module, we can from these numbers calculate the probability that the eight teams would come from the actual conference should have occurred by chance (from the hypergeometrical distribution), and the same probability for the two teams from the other conference. These probabilities are the p-values for this instance, and we assign the lowest one we find to this module. For future processing, we store the negative logarithm of this p-value.

4 For reasons that will become clear in the next section, we do not calculate the total probability for this event.
However, it is problematic to consider these $p$-values as true probabilities since there are many different tests we perform (one for each class of nodes which exists within the actual module), i.e., this is a multiple testing problem. It is likely that unlikely things should occur. Therefore we pick eleven random teams and calculate the $p$-values in the same way again, keeping the lowest one. By repeating this many times, we obtain a distribution of (negative logarithms of) $p$-values which has a mean, $\bar{p}$, and a standard deviation, $\sigma_p$. From this, we can construct standard $Z$-scores as

$$Z = \frac{p - \bar{p}}{\sigma_p}$$ \hspace{1cm} (9)

These $Z$-scores indicate how unlikely the present distribution is, such that the higher $Z$-score, the more improbable the actual distribution, and the more relevance our found module has. That is, they form a coherence score for the community.

By considering all modules simultaneously, and proceeding in the way described above, we obtain a global coherence score for the whole community structure. In Fig. 7, we show the modularity, the distances from the true partition (both $m_{\text{moved}}$ and $m_{\text{div}}$) and the coherence-scores for different number of communities. The algorithms employed are hierarchical clustering (shortest path) in (a) and (c), and K-means (sum of paths) in (b) and (d). We clearly see how the coherence score and the modularity co-vary, such that they essentially peak at the same number of clusters. Remembering that the modularity is a graph-theoretical measure relying only on network properties (paying no attention to what the nodes represent) and that the coherence score does not utilize that the underlying structure is a network but only focus on the annotations of the nodes, this is a remarkable result. Further, we see in (c) and (d) how the total distances, both $m_{\text{moved}}$ and $m_{\text{div}}$, have minima approximately where the modularity peaks. These observations support the tacit assumption in many previous papers that the partition with the highest modularity also corresponds to the one that makes most sense.

6 Gene network of *Saccharomyces cerevisiae*

As our final example, we consider a somewhat larger network where no true partition exists (or at least is known). The network represents the interactions between regulatory proteins and genes in *Saccharomyces cerevisiae* (ordinary yeast) [17]. The 690 nodes represent genes, and the 1079 edges correspond to biochemical interactions. The edges are directed from a gene that encodes for a transcription factor to a gene transcriptionally regulated by that protein, i.e., we have a directed network. However, here we remove all directionality from the edges in order to more easily apply the same algorithms and measures as before in this paper.

A few are “pseudogenes”, which here means that they are complexes, composed by two or more gene products.
We have partitioned this gene network into several communities using the algorithms described above. For each number of communities, we have as before calculated the modularity (4) and the coherence (9), see Fig. 8.

![Fig. 8. Modularity (solid curve) and coherence (dashed curve) for the communities detected in the gene network of Saccharomyces cerevisiae. The coherence is scaled down with a factor of 100. Left: Hierarchical clustering (shortest path). Right: K-means clustering (sum of paths).](image)

The external validation for calculating the coherence is this time somewhat less straightforward. We employ the Gene Ontology (GO) database [1] in order to find a classification for the nodes genes of the network. In this database, the genes of S. cerevisiae (and several other organisms) are arranged in a directed acyclic graph according to which biological process they belong. A gene is assigned both the ontology term for the process it belongs to, as well as all terms for the parental processes in the graph, i.e., there are many different terms associated with each gene. To judge the quality of a specific community partitioning, we query the database with a list of all genes in each community. It is because of these multiple annotations of all genes we cannot calculate one probability for the whole network division, as remarked in the previous section. These p-values are then treated the same way as for the football teams, and we obtain coherence scores from the same kind of null hypothesis as before. In Fig. 9 we show the distribution of all coherence scores for the divisions into 22 and 177 communities, respectively, obtained by hierarchical clustering (shortest path), with corresponding Q-values of $Q = 0.67$ and $Q = 0.51$ (see Fig. 8).

This time, we cannot measure the distance from any kind of “true” partition. Instead we do a pairwise comparison between different methods. In Fig. 10 we show the normalized total distances $\hat{m}_{\text{moved}}$ and $\hat{m}_{\text{div}}$ between some different partition-

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6 They can also be ordered according to biological function or cellular localization, properties we do not utilize here.

7 Without prior knowledge of the network, it is hard to tell whether a distance is small or large just from the numbers $m_{\text{moved}}$ and $m_{\text{div}}$. Therefore, we normalize these numbers by dividing them by the distances obtained as the mean of a sample of random partitionings with the same number of clusters and the same number of units in each cluster as for the
Fig. 9. Coherence scores (Z-values) for the biological process terms, associated to each community. The light grey bars correspond to a division into 22 communities obtained with hierarchical clustering (shortest path) and has $Q = 0.67$. The dark grey bars correspond to 177 communities, obtained with the same algorithm and with $Q = 0.51$. The widths of the bars are proportional to the number of genes in each community.

Fig. 9 shows the normalized distances between the very “best” (highest modularity) division obtained with K-means (shortest path) and the divisions obtained by the same algorithm for the number of communities depicted along the x-axis. To the right, the figure shows the normalized distances between the partitioning obtained by hierarchical clustering (shortest path) and the one obtained by K-means (shortest path), for the number of communities depicted along the x-axis. Remarkably, we see how these distances have their minima not far from where the modularity and the coherence score have their peaks. By definition, the minima in the left panel have to be exactly zero, but worth noting is how sharp these extrema are. The minima in the right panel are broader, but still in a clear neighbourhood of the maxima of the modularity and the coherence score. The conclusion is that the outcome of the different clustering algorithms seem to coincide, as long as we are satisfied with looking at the “best” partition (in the sense of having the highest modularity). However, if we for some reason do not strive for this optimum, the procedures can give rise to very different results.
Fig. 10. Normalized total distance between the very best division obtained by K-means (shortest path) and K-means (shortest path) with a various number of communities (depicted at the x-axis) (left), and between partitionings obtained by hierarchical clustering (shortest path) and K-means (shortest path) for the same number of communities (right). Solid (upper) curves are $\tilde{m}_{\text{moved}}$, while the dashed (lower) curves are $\tilde{m}_{\text{div}}$.

7 Discussion and conclusions

We have in the present article presented various aspects of how to find and evaluate community structures in complex networks. The issue of finding such a structure is closely related to clustering of data based on similarity over many experiments, without any underlying network structure assumed. This latter exploration is a standard tool today, and there are many well-developed algorithms for handling the issue. Here we show explicitly that at least some of these algorithms can be used also for finding communities, indeed, one of them provided the best partitioning in terms of high modularity we have found in the literature thus far. A drawback, however, is that these algorithms are computationally less efficient.

Since there is no generally accepted definition of what really constitutes a reasonable partitioning, we explored both Newman’s modularity and the so-called Silhouette index. The former has become some kind of de-facto standard, and many authors simply equate a proposed modular structure with having a high modularity. As a contrast, we also investigated the Silhouette index, but found rapidly that it was less suitable for networks.

The question of how distant two partitionings of the same network are is somewhat new in the present physics literature, although the issue by no means is original. We described two different such measures and discussed advantages and drawbacks of each. A combined use of both yields of course a better description. We also turned these to measure into indices and compared them with the Jaccard index and the mutual information index, showing that the behaviour was similar among

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8 To the best of our knowledge, the only exception is [4], which one of the referees draw our attention to.
Finally, we proposed the introduction of a coherence score, indicating the validity of the partitioning. This score is especially well-suited when each node in network has several annotations, or belongs to annotations presented as a directed acyclic graph, where children inherit all the parents’ annotations. This is the case for the Gene Ontology database, which has become very popular recently in the bioinformatics community. It turns out that the modularity and the coherence score peak for approximately the same number of communities, at least for the networks we have considered here. Hence, this observation gives support to the standard procedure of only striving for optimizing the modularity.

In summa, the issue of finding and evaluating community structures in complex networks is an important part in the unraveling of properties for the systems. Here we have discussed various aspects of these themes, and also introduced the new concept of “coherence” for a network. We strongly believe this can be a valuable tool in the future for the exploration of various networks.

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