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Detecting the overlapping and hierarchical community structure in complex networks

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Abstract. Many networks in nature, society and technology are characterized by a mesoscopic level of organization, with groups of nodes forming tightly connected units, called communities or modules, that are only weakly linked to each other. Uncovering this community structure is one of the most important problems in the field of complex networks. Networks often show a hierarchical organization, with communities embedded within other communities; moreover, nodes can be shared between different communities. Here, we present the first algorithm that finds both overlapping communities and the hierarchical structure. The method is based on the local optimization of a fitness function. Community structure is revealed by peaks in the fitness histogram. The resolution can be tuned by a parameter enabling different hierarchical levels of organization to be investigated. Tests on real and artificial networks give excellent results.

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1. Introduction

The study of networks as the ‘scaffold of complexity’ has proved very successful to understand both the structure and the function of many natural and artificial systems [1]–[5]. A common feature of complex networks is community structure [6]–[9], i.e. the existence of groups of nodes such that nodes within a group are much more connected to each other than to the rest of the network. Modules or communities reflect topological relationships between elements of the underlying system and represent functional entities. For example, communities may be groups of related individuals in social networks [6, 10, 11], sets of web pages dealing with the same topic [12], taxonomic categories in food webs [13, 14], biochemical pathways in metabolic networks [15]–[17], etc. Therefore the identification of communities is of central importance, but it has remained a formidable task.

The solution is hampered by the fact that the organization of networks at the ‘mesoscopic’, modular level is usually highly nontrivial, for at least two reasons. First, there is often a whole hierarchy of modules, because communities are nested: small communities build larger ones, which in turn group together to form even larger ones, etc. An example could be the organization of a large firm, and it has been argued that the complexity of life can also be mapped to a hierarchy of networks [18]. The hierarchical form of organization can be very efficient, with the modules taking care of specific functions of the system [19]. In the presence of hierarchy, the concept of community structure becomes richer, and demands a method that is able to detect all modular levels, not just a single one. Hierarchical clustering is a well-known technique in social network analysis [20, 21], biology [22] and finance [23]. Starting from a partition in which each node is its own community, or all nodes are in the same community, one merges or splits clusters according to a topological measure of similarity between nodes. In this way, one builds a hierarchical tree of partitions, called a dendrogram. Though this method naturally produces a hierarchy of partitions, nothing is known a priori about their qualities. The modularity of Newman and Girvan [24] is a measure of the quality of a partition, but it can identify a single partition, i.e. the one corresponding to the largest value of the measure. Only recently have scholars started to focus on the problem of identifying meaningful hierarchies [19, 25].

A second difficulty is caused by the fact that nodes often belong to more than one module, resulting in overlapping communities [17], [26]–[29]. For instance, people belong to different social communities, depending on their families, friends, professions, hobbies, etc. Nodes belonging to more than one community are a problem for standard methods and lower the quality of the detected modules. Moreover, this conceals important information, and often leads to misclassifications. The problem of overlapping communities was exposed in [17], where a solution to it was also offered. The proposed method is based on clique percolation: a $k$-clique (a complete subgraph of $k$ nodes) is rolled over the network through other cliques with $k - 1$ common nodes. In this way a set of nodes can be reached, which is identified as a community. One node can participate in more than one such unit, therefore overlaps naturally occur. The method, however, is not suitable for the detection of hierarchical structure, as once the size $k$ of the clique is specified, mostly a single modular structure can be recovered. In figure 1, we show distinct networks with hierarchical structure and overlapping communities, though it should be emphasized that these features often occur simultaneously.

In order to provide the most exhaustive information about the modular structure of a graph, a good algorithm should be able to detect both overlapping communities and hierarchies between them. In this paper, we introduce a framework that accomplishes these two demands.
Figure 1. Top: a network with a hierarchical structure. Each of the four large clusters is made out of 128 nodes and has an internal subdivision in four clusters with 32 nodes. Bottom: overlapping communities. The green nodes are topologically related to more groups.

The method performs a local exploration of the network, searching for the natural community of each node. During the procedure, nodes can be visited many times, no matter whether they have been assigned to a community or not. In this way, overlapping communities are naturally recovered. The variation of a resolution parameter, determining the average size of the communities, allows all hierarchical levels of the network to be explored.

2. The method

The basic assumption behind our algorithm is that communities are essentially local structures, involving the nodes belonging to the modules themselves plus at most an extended neighborhood of them. This is certainly plausible for large networks, where each node does not depend on most of its peers. In the link graph of the WWW, for instance, one does not even have a perception of how large the network is, and topical communities are formed based only on partial information about the graph. Similarly, social communities are local structures without any reference to humankind as a whole.

Here, a community is a subgraph identified by the maximization of a property or fitness of its nodes. We have tried several options for the form of the fitness and obtained the best results with the simple expression

$$f_G = \frac{k_{in}^G}{(k_{in}^G + k_{out}^G)\alpha},$$  

(1)
where $k_{\text{in}}^G$ and $k_{\text{out}}^G$ are the total internal and external degrees of the nodes of module $G$, and $\alpha$ is a positive real-valued parameter, controlling the size of the communities. The internal degree of a module equals double the number of internal links of the module. The external degree is the number of links joining each member of the module with the rest of the graph. The aim of this paper is to determine a subgraph starting from node $A$ such that the inclusion of a new node, or the elimination of one node from the subgraph would lower $f_G$. We call such a subgraph the natural community of node $A$. This amounts to determining local maxima for the fitness function for a given $\alpha$. The true maximum for each node trivially corresponds to the whole network, because in this case $k_{\text{out}}^G = 0$ and the value of $f_G$ is the largest that the measure can possibly attain for a given $\alpha$. The idea of detecting communities by a local optimization of some metric has already been applied earlier [26, 27, 30, 31].

It is helpful to introduce the concept of node fitness. Given a fitness function, the fitness of a node $A$ with respect to a subgraph $G$, $f_A^G$, is defined as the variation of the fitness of the subgraph $G$ with and without node $A$, i.e.

$$f_A^G = f_{G+\{A\}} - f_{G-\{A\}}. \tag{2}$$

In equation (2), the symbol $G + \{A\}$ ($G - \{A\}$) indicates the subgraph obtained from module $G$ with node $A$ inside (outside).

The natural community of node $A$ is identified with the following procedure. Let us suppose that we have covered a subgraph $G$ including node $A$. Initially, $G$ is identified with node $A$ ($k_{\text{in}}^G = 0$). Each iteration of the algorithm consists of the following steps:

1. a loop is performed over all neighboring nodes of $G$ not included in $G$;
2. the neighbor with the largest fitness is added to $G$, yielding a larger subgraph $G'$;
3. the fitness of each node of $G'$ is recalculated;
4. if a node turns out to have negative fitness, it is removed from $G'$, yielding a new subgraph $G''$;
5. if 4 occurs, repeat from 3, otherwise repeat from 1 for subgraph $G''$.

The process stops when the nodes examined in step 1 all have negative fitness (figure 2). This procedure corresponds to a sort of greedy optimization of the fitness function, as at each move one looks for the highest possible increase. Other recipes may be adopted as well. For instance, one could backtrack nodes with negative fitness only when the cluster stops growing and/or include in the cluster the first neighboring node that produces an increase of the fitness. Such recipes may lead to higher fitness clusters in a shorter time, and deserve in-depth investigations, which we leave for future work.

We define a cover of the graph as a set of clusters such that each node is assigned to at least one cluster. This is an extension of the traditional concept of graph partition (in which each node belongs to a single cluster), to account for possible overlapping communities. In our case, detecting a cover amounts to discovering the natural community of each node of the graph being studied. The straightforward way to achieve this is to repeat the above procedure for each single node. This is, however, computationally expensive. The natural communities of many nodes often coincide, so most of the computer time is spent on rediscovering the same modules again and again. An economic way out can be summarized as follows:

1. pick a node $A$ at random;
2. detect the natural community of node $A$;
Figure 2. Schematic example of natural community for a node (sky-blue point in the figure) according to our definition. The blue nodes are the other members of the group and have positive fitness within the group, while the red nodes have all negative fitness with respect to the group.

3. pick at random a node $B$ not yet assigned to any group;
4. detect the natural community of node $B$, exploring all nodes regardless of their possible membership to other groups;
5. repeat from 3.

The algorithm stops when all nodes have been assigned to at least one group. Our recipe is justified by the following argument. The nodes of every community either overlap with other communities or not. The community was explored around a specific node; if one chose any one of the other nodes, one would either recover the same community or one of the possible overlapping communities. But the latter can be found as well if one starts from nodes that are outside the community at hand and non-overlapping with it. In this way, one should recover all modules without needing to start from every node. At the same time, overlapping nodes will be covered during the construction of each community they belong to, as it is possible to include nodes already assigned to other modules. Extensive numerical tests show that the loss in accuracy is minimal if one proceeds as we suggest rather than by finding the natural community of all nodes. We remark that the procedure has some degree of stochasticity, due to the random choice of the node seeds from which communities are closed. This issue is discussed in appendix A.

The parameter $\alpha$ tunes the resolution of the method. Fixing $\alpha$ means setting the scale at which we are looking at the network. Large values of $\alpha$ yield very small communities, small values instead deliver large modules. If $\alpha$ is small enough, all nodes end up in the same cluster, the network itself. We have found that, in most cases, for $\alpha < 0.5$, there is only one community; for $\alpha > 2$, one recovers the smallest communities. A natural choice is $\alpha = 1$, as it is the ratio of the external degree to the total degree of the community. This corresponds to the so-called weak definition of community introduced by Radicchi et al [32]. We found that, in most cases, the cover found for $\alpha = 1$ is relevant, so it gives useful information about the actual community.
structure of the graph in question. Sticking to a specific value of $\alpha$ means constraining the resolution of the method, much as happens by optimizing Newman–Girvan’s modularity [33, 34]. However, one cannot know a priori how large the communities are, as this is one of the unknowns of the problem, so it is necessary to compare covers obtained at different scales.

By varying the resolution parameter one explores the whole hierarchy of covers of the graph, from the entire network down to the single nodes, leading to the most complete information on the community structure of the network. However, the method also gives a natural way to rank covers based on their relevance. It is reasonable to think that a good cover of the network is stable, i.e. it can be destroyed only by changing appreciably the value of $\alpha$ for which it was recovered. Each cover is delivered for $\alpha$ lying within some range. A stable cover would be indicated by a large range of $\alpha$. What we need is a quantitative index to label a cover $P$. We shall adopt the average value $\bar{f}_P$ of the fitness of its communities, i.e.

$$\bar{f}_P = \frac{1}{n_c} \sum_{i=1}^{n_c} f_{G_i}(\alpha = 1),$$

where $n_c$ is the number of modules. The fitness must be calculated for a fixed value of $\alpha$ (we choose $\alpha = 1$ for simplicity), such that identical (different) covers can be recognized by equal (different) values. We shall derive the histogram of the $\bar{f}_P$-values of the covers obtained for different $\alpha$-values: stable covers are revealed by pronounced peaks in the resulting fitness histogram. The higher the peak, the more stable the cover. In this way, covers can be ranked based on their frequency. A similar concept of stability has been adopted in a recent study, where a resolution parameter was introduced in Newman–Girvan’s modularity [35].

A natural question is how to combine hierarchical communities with overlapping communities, as the usual meaning of hierarchy seems incompatible with the existence of nodes shared among communities. However, this is only apparent and the same definition of hierarchical partitions can be extended to the case of overlapping communities. We say that two covers $C'$ and $C''$ are hierarchically ordered, with $C'$ higher than $C''$, if all nodes of each community of $C''$ participate (fully or partially) in a single community of cover $C'$.

It is hard to estimate the computational complexity of the algorithm, as it depends on the size of the communities and the extent of their overlaps, which in turn strongly depends on the specific network being studied along with the value of the parameter $\alpha$. The time to build a community with $s$ nodes scales approximately as $O(s^2)$, due to the backtracking steps. Therefore, a rough estimate of the complexity for a fixed $\alpha$-value is $O(n_c(s^2))$, where $n_c$ is the number of modules of the delivered cover and $\langle s^2 \rangle$ the second moment of the community size. The square comes from the loop over all nodes of a community to check for their fitness after each move. The worst-case complexity is $O(n^2)$, where $n$ is the number of nodes of the network when communities are of size comparable with $n$. This is in general not the case, so in most applications the algorithm runs much faster and almost linearly when communities are small. The situation is shown in figure 3, where we plot the time to run the algorithm to completion for two different $\alpha$-values as a function of the number of nodes for Erdős–Rényi graphs with an average degree of 10: the complexity goes from quadratic to linear. The total complexity of the algorithm to perform the complete analysis of a network also depends on the number of $\alpha$-values required to resolve its hierarchical structure. The better the hierarchy of covers can be displayed, the larger the number of $\alpha$-values used to run the algorithm. If the network has a hierarchical structure, as often happens in real systems, the number of covers grows as $\log n$. In this case, the number of different $\alpha$-values required to resolve the hierarchy is also of the order...
of \( \log n \) and the complete analysis can be carried out very quickly. We note that each iteration of the algorithm for a given \( \alpha \) is independent of the others. So, the calculation can be trivially parallelized by running different \( \alpha \)-values on each computer. If large computer resources are not available, a cheap way to proceed could be to start from a large \( \alpha \)-value, for which the algorithm runs to completion in a very short time, and use the final cover as the initial configuration for a run at a slightly lower \( \alpha \)-value. Since the corresponding cover is similar to the initial one, the second run would also be completed in a short time and one can repeat the procedure all the way to the left of the range of \( \alpha \).

We conclude that for hierarchical networks our procedure has a worst-case computational complexity of \( O(n^2 \log n) \). We remark that, if it is true that several algorithms nowadays have a lower complexity, none of them are capable of carrying out a complete analysis of the hierarchical community structure, as they usually deliver a single partition. Therefore a fair comparison is not possible. Besides, other recipes for the local optimization of our or other fitness functions may considerably lower the computational complexity of the algorithm, which seems a promising research direction for the future.

3. Results

We extensively tested our method on artificial networks with built-in hierarchical community structure. We adopted a benchmark similar to that recently proposed by Arenas et al \([36, 37]\), which is a simple extension of the classical benchmark proposed by Girvan and Newman \([6]\). There are 512 nodes, arranged in 16 groups of 32 nodes each. The 16 groups are ordered into four supergroups. Every node has an average of \( k_1 \) links with the 31 partners of its group and \( k_2 \) links with the 96 nodes of three other groups within the same supergroup. In addition, each
The normalized mutual information is used to compare the cover found by the algorithm with the natural cover of the network at each level. At the higher level (circles), the communities are four clusters each including 32 nodes, for a total of 128 nodes per cluster. Our method finds the right clusters as long as they are not well mixed with each other. At the lower level (squares), the communities are 16 clusters of 32 nodes each. The method performs very well, considering that each node has as many links inside as outside each micro-community, for any value of $k_3$. The dashed vertical line marks the graph configurations for which the number of links of each node within its macro-community equals the number of links connecting the node to the other three macro-communities.

We have to check whether the built-in hierarchy is recovered through the algorithm. This, in general, depends on the parameter $k_3$. Therefore, we considered different values of $k_3$: for each value, we built 100 realizations of the network. To compare the built-in modular structure with the one delivered by the algorithm, we adopt the normalized mutual information, a measure of similarity borrowed from information theory, which has proved to be reliable [38]. The extension of the measure to overlapping communities is not trivial and there are several alternatives. Our extension is discussed in appendix B. In figure 4, we plot the average value of the normalized mutual information as a function of $k_3$ for the two hierarchical levels. We see that in both cases the results are very good. The cover in the four supergroups or macro-communities is correctly identified for $k_3 < 24$, with very few exceptions, and the algorithm starts to fail only when $k_3 \sim 32$, i.e. when each node has 32 links inside and 32 outside of its macro-community, which is then mixed well with the others. The performance is very good as well for the lower
Figure 5. Analysis of real networks. The fitness histograms correspond to Zachary’s karate club (top-left panel), Lusseau’s dolphins’ network (top-right panel) and the network of American college football teams (bottom-left panel). The highest peaks indicate the best covers, which coincide with the natural covers of the graphs, except for Zachary’s karate club, where it corresponds to the same split in four clusters found through modularity optimization. However, the social cover in two of the networks is the third most relevant cover. In the bottom-right panel, we show the fitness histogram for an Erdős–Rényi random graph with 100 nodes and the same average degree as the network of American college football teams: there is no visible structure, as expected.
Figure 6. (a) Zachary’s karate club. We show the hierarchical levels corresponding to the cover in two clusters ($0.76 < \alpha < 0.84$). The nodes 3, 9, 10, 14 and 31 are shared between the two groups: such nodes are often misclassified by traditional algorithms. The non-overlapping nodes reflect the social fission observed by Zachary, which is illustrated by the squares and the circles in the figure. (b) Lusseau’s network of bottlenose dolphins. The best cover in two clusters that we found ($0.77 < \alpha < 0.82$) agrees with the separation observed by Lusseau (squares and circles in the figure). The nodes 8, 20, 29, 31 and 40 are shared between the two groups.

Sound, New Zealand. The network was studied by the biologist David Lusseau, who divided the dolphins into two groups according to their age. The third example is the network of American college football teams. Here, there are 115 nodes, representing the teams, and two nodes are connected if their teams play against each other. The teams are divided into 12 conferences. Games between teams in the same conference are more frequent than games between teams of different conferences, so one has a natural cover where the communities correspond to the conferences.

The pronounced spikes in the histograms of figure 5 show that these networks indeed have community structure. For Zachary’s network, we find that the most stable cover consists of four clusters. Even if this is not what one would like to recover, we stress that this cover is often found by other methods, like modularity optimization, which indicates that it is topologically meaningful. But our method can do better: the social split in two clusters (figure 6(a)) turns out to be a higher hierarchical level, given by a pairwise merging of the four communities.
Figure 7. Fraction of overlapping nodes as a function of $\alpha$ for the three real networks discussed in figure 5: Zachary’s karate club and the networks of dolphins and American football teams. There is no unique pattern, the extent of the overlap does not show a systematic variation with $\alpha$.

of the main cover. Interestingly, we found that the two groups are overlapping, sharing a few nodes. For the dolphins’ network, the highest spike corresponds to Lusseau’s subdivision of the animals’ population in two communities, with some overlap between the two groups (figure 6(b)). Similarly, the highest spike in figure 5 (bottom-left panel) corresponds to the natural partition of the teams in conferences.

To check how good our algorithm performs as compared to other methods, we have analyzed the karate, dolphins and American college football networks with the clique percolation method (CPM) of Palla et al [17]. The values of the normalized mutual information of the covers found by the algorithm with respect to the real covers are 0.690 (our method) and 0.170 (CPM) for the karate club, 0.781 (our method) and 0.254 (CPM) for the dolphins’ network, and 0.754 (our method) and 0.697 (CPM) for the American college football network. So our method proves superior to the CPM in these instances. On the other hand, the CPM performs better for networks with many cliques. An example is represented by the word association network built on the University of South Florida Free Association Norms [41], analyzed in [17]. The CPM finds groups of words that correspond to well-defined categories, whereas with our method the categories are more mixed. An important reason for this discrepancy is that our method recovers overlapping nodes that usually lie at the border between communities, whereas in the word association network they are often central nodes of a community. For instance, the word ‘color’ is the central hub of the community of colors, but it also belongs to other categories like ‘astronomy’ and ‘light’.

We performed tests on many other real systems, including protein interaction networks, scientific collaboration networks and other social networks. In all cases, we found reasonable covers. On the other hand, we found that random graphs have no natural community structure, as covers are unstable (figure 5 (bottom-right panel)). This is remarkable, as it is known that other approaches may find covers in random graphs as well [42], a problem that triggered an ongoing debate as to when a cover is indeed relevant [43].
In figure 7, we show how the extent of the overlap between the communities depends on the resolution parameter $\alpha$, for three real networks. From the figure it is not possible to infer any systematic dependence of the overlap on $\alpha$, the pattern is strongly dependent on the specific graph topology.

We conclude the section with an analysis of the statistical properties of community structure in graphs. Figure 8 shows the distribution of community sizes for a sample of the WWW link graph, corresponding to the subset of Web pages within the domain.gov. We analyzed the largest connected component of the graph, consisting of 774,908 nodes and 4,711,340 links. The figure refers to the cover found for $\alpha = 1$, which was identified within less than 40 h of CPU time on a small PC. The distribution of community sizes is skewed, with a tail that follows a power law with exponent 2.2 (dashed line in the figure). The result is consistent with previous analyses of community size distributions on large graphs [8, 17, 44, 45], although this is the first result concerning the WWW. We stress that we have not performed a complete analysis of this network, because it would require a lot of processors to carry out the high number of runs at different $\alpha$-values which are necessary for a reliable analysis. Therefore, the distribution in figure 8 does not necessarily correspond to the most significant cover. However, the $\alpha$-values of the most representative covers of all networks we have considered turned out to be close to 1, so the plot of figure 8 is likely to be a fair approximation of the actual distribution.

4. Conclusions

In this paper, we have presented the first method that uncovers simultaneously both the hierarchical and the overlapping community structure of complex networks. The method consists of finding the local maxima of a fitness function by local, iterative searching. The procedure enables each node to be included in more than one module, leading to a natural
description of overlapping communities. Finally, by tuning the resolution parameter $\alpha$ one can probe the network at different scales, exploring the possible hierarchy of community structure. The application of our method to a number of constructed and empirical networks has given excellent results.

We would like to emphasize that our method provides a general framework that yields a large class of algorithms. For instance, one could choose a different expression for the fitness function, another criterion to define the most meaningful cover, or a different optimization procedure of the fitness for a single cluster. The setup we have tested proves to be very reliable, but we cannot exclude that different choices yield even better results. In fact, the framework is so flexible that it can be easily adapted to the problem at hand: if one has hints about the topology of the communities to be found for a specific system, this information can be used to design a particular fitness function, accounting for the required features of the modules.

Since the complete analysis of a network’s community structure can be carried out simultaneously on many computers, the upper size limit of tractable graphs can be pushed up considerably. Our method gives the opportunity to study systematically the distribution of community sizes of large networks up to millions of nodes, a crucial aspect of the internal organization of a graph, which scholars have just begun to examine. An interesting by-product of our technique is the possibility of quantifying the participation of overlapping nodes in their communities by the values of their (node) fitness with respect to each group they belong to.

Finally, we would like to mention that the method can be naturally extended to weighted networks, i.e. networks where links carry a weight. There is no need to use any kind of thresholding [46], as the generalization of the fitness formula is straightforward: in equation (1), we have to replace the degree $k$ with the corresponding strength $s$ (expressing the sum over the links’ weights). Applications to directed networks can also be easily devised with suitable choices of the fitness function. Our own function (1) could be extended to the directed case, in that one considers the indegree of the nodes of a subgraph: it is plausible to assume that the total indegree of the nodes of the subgraph due to links internal to the subgraph exceeds the total indegree produced by links coming from external nodes, if the subgraph is a community.

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Appendix A. Dependence on the random seeds

The choice of the random seeds where the community exploration starts may affect covers obtained for the same $\alpha$-value. This means, in principle, that we cannot rely on the fitness histogram found for a specific choice of the seeds. We have found that covers obtained for different seeds are quite close to each other, and that the most relevant covers that emerge from the analysis are the same for any choice of the seeds. What may depend on the specific seed adopted is the ranking of the covers. This can be solved by performing some additional runs of the algorithm for different seeds in correspondence to the regions of the $\alpha$-range in which meaningful structures have been spotted after the first scan. The final ranking of the covers is then more reliable than any ranking obtained for a specific choice of the random seeds. Since
the number of relevant peaks is much smaller than the number of nodes \( n \), the computational cost of the additional runs is negligible as compared to the total number of runs.

**Appendix B. Comparing partitions**

The aim of this section is to discuss the problem of comparing covers. There are many criteria in the literature (see [47]), but, to the best of our knowledge, the case of overlapping clusters has not been considered yet. Here, we briefly discuss the issue within the framework of information theory [48].

The normalized mutual information \( I_{\text{norm}}(X : Y) \) [38] is defined as

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

where \( H(X) (H(Y)) \) is the entropy of the random variable \( X \) (\( Y \)) associated with the partition \( C' \) (\( C'' \)), whereas \( H(X, Y) \) is the joint entropy. This variable is in the range \([0, 1]\) and equals 1 only when the two partitions \( C' \) and \( C'' \) are exactly coincident. Another possible similarity measure is the variation of information \( V(X, Y) = H(X|Y) + H(Y|X) \) [43, 47]. One way to normalize \( V(X, Y) \) is

\[
V_{\text{norm}}'(X, Y) = \frac{1}{2} \left( \frac{H(X|Y)}{H(X)} + \frac{H(Y|X)}{H(Y)} \right),
\]

which can be interpreted as the average relative lack of information to infer \( X \) given \( Y \) and vice versa. This normalization will be helpful in the following.

Let us now suppose that a node may belong to more than one cluster. The membership of the node \( i \) is not a number \( x_i \in \{1, 2 \ldots |C'|\} \) anymore, but it must be considered as a binary array of \(|C'|\) entries, one for each cluster of the partition \( C' \) (say \((x_i)_k = 1 \) if the node \( i \) is present in the \( C'_k \) cluster, \((x_i)_k = 0 \) otherwise). We can regard the \( k \)th entry of this array as the realization of a random variable \( X_k = (X)_k \), whose probability distribution is

\[
P(X_k = 1) = n_k / N, \quad P(X_k = 0) = 1 - n_k / N,
\]

where \( n_k \) is the number of nodes in the cluster \( C'_k \) of \( C' \), i.e. \( n_k = |C'_k| \). The same holds for the random variable \( Y_k \) associated with the cluster \( C''_k \) of \( C'' \).

It is possible to define the joint distribution \( P(X_k, Y_k) \) :

\[
P(X_k = 1, Y_k = 1) = \frac{|C'_k \cap C''_k|}{N},
\]

\[
P(X_k = 1, Y_k = 0) = \frac{|C'_k| - |C'_k \cap C''_k|}{N},
\]

\[
P(X_k = 0, Y_k = 1) = \frac{|C''_k| - |C'_k \cap C''_k|}{N},
\]

\[
P(X_k = 0, Y_k = 0) = \frac{N - |C'_k \cup C''_k|}{N}.
\]
Again, we want to define how similar \(C'\) and \(C''\) are in terms of lack of information about one cover given the other. In particular, we can define the amount of information to infer \(X_k\) given a certain \(Y_l\)

\[
H(X_k | Y_l) = H(X_k, Y_l) - H(Y_l). \tag{B.8}
\]

In order to infer \(X_k\), we can choose one \(Y_l\) among \(|C''|\) possible candidates. In particular, if a cluster \(C''_b\) of \(C''\) turns out to be the same as \(C'_k\), we have that \(H(X_k | Y_b) = 0\), and we would like to say that \(Y_b\) is the best candidate to infer \(X_k\). So, in a set matching fashion, we can decide to consider only \(Y_b\) and neglect all the other variables \(Y_l\). In particular, we can define the conditional entropy of \(X_k\) with respect to all the components of \(Y\),

\[
H(X_k | Y) = \min_{l \in \{1, 2, \ldots, |C''|\}} H(X_k | Y_l). \tag{B.9}
\]

As in equation (B.2), we can normalize \(H(X_k | Y)\) dividing by \(H(X_k)\)

\[
H(X_k | Y)_{\text{norm}} = \frac{H(X_k | Y)}{H(X_k)} \tag{B.10}
\]

and taking the average over \(k\) eventually leads to the definition of the normalized conditional entropy of \(X\) with respect to \(Y\),

\[
H(X | Y)_{\text{norm}} = \frac{1}{|C'|} \sum_k \frac{H(X_k | Y)}{H(X_k)}. \tag{B.11}
\]

The expression for \(H(Y | X)_{\text{norm}}\) can be determined in the same way. So, we can finally define

\[
N(X | Y) = 1 - \frac{1}{2} [H(X | Y)_{\text{norm}} + H(Y | X)_{\text{norm}}]. \tag{B.12}
\]

The function \(N(X | Y)\) has the appealing property of being equal to one if and only if \(X_k = f(Y_l)\) for a certain \(l\), and vice versa. Unfortunately, this does not imply that \(C'\) and \(C''\) are equal. In particular, it may happen that \(X_k\) is the negative of \(Y_l\), i.e.

\[
|C'_k \cap C''_l| = 0 \quad \text{and} \quad |C'_k \cup C''_l| = N. \tag{B.13}
\]

In this case, we do not need additional information about \(X_k\) if we know \(Y_l\) because we are sure that if a node belongs to \(C''_l\) it does not belong to \(C'_k\) and vice versa; nevertheless, the two covers are not equal. In other words, taking the minimum in equation (B.9) may not imply choosing a cluster \(C''_b\) very similar to \(C'_k\): a cluster that is close to the complementary of \(C'_k\) can be a good candidate as well.

To avoid this problem, we add a constraint in equation (B.9): the only eligible \(Y_l\) are those ones which are far from being the negatives of \(X_k\), i.e. those fulfilling the following condition:

\[
h[P(1, 1)] + h[P(0, 0)] > h[P(0, 1)] + h[P(1, 0)], \tag{B.14}
\]
where we used the short notation $P(1, 1) = P(X_k = 1, Y_l = 1)$ and $h(p) = -p \log p$. To understand why this constraint is appropriate, let us write explicitly the conditional entropy (equation (B.8))

$$H(X_k|Y_l) = h[P(1, 1)] + h[P(0, 0)] + h[P(0, 1)] + h[P(1, 0)] - h[P(Y_l = 1)] - h[P(Y_l = 0)].$$ (B.15)

In the case of $C''$ equal to $C'$, we have

$$h[P(1, 1)] = h[P(Y_l = 1)] \quad \text{and} \quad h[P(0, 0)] = h[P(Y_l = 0)],$$ (B.16)

while the mixing terms vanish

$$h[P(0, 1)] = 0 \quad \text{and} \quad h[P(1, 0)] = 0.$$ (B.17)

On the other hand, if $C'$ is the complementary to $C'$, the role of $h(P(1, 1))$ and $h(P(0, 0))$ is played by the mixing terms:

$$h[P(0, 1)] = h[P(Y_l = 1)] \quad \text{and} \quad h[P(1, 0)] = h[P(Y_l = 0)],$$ (B.18)

while

$$h[P(1, 1)] = 0 \quad \text{and} \quad h[P(0, 0)] = 0.$$ (B.19)

So, in the former case all the information quantified by $H(X_k, Y_l)$ is used to encode the positive cases, i.e. $H(X_k, Y_l) = h[P(1, 1)] + h[P(0, 0)]$, while in the latter it is used to encode the mixing terms, i.e. $H(X_k, Y_l) = h[P(1, 0)] + h[P(0, 1)]$. Then, the condition expressed by equation (B.14) means that more than one-half of $H(X_k, Y_l)$ is used to encode the positive cases, and so it excludes the clusters close to being complementary.

If none of the $Y_l$ fulfills equation (B.14), we set

$$H(X_k|Y) = H(X_k).$$ (B.20)

All this assures that $N(X|Y) = 1$ if and only if the two covers $C'$ and $C''$ are equal.

To sum up, all the procedure reduces to

1 for a given $k$, compute $H(X_k|Y_l)$ for each $l$ using the probabilities given by equations (B.4)–(B.7);

2 compute $H(X_k|Y)$ from equation (B.9) taking into account the constraint given in equation (B.14); note that if this condition is never fulfilled, we decided to set $H(X_k|Y) = H(X_k)$;

3 for each $k$, repeat the previous step to compute $H(X|Y)_{\text{norm}}$ according to equation (B.11);

4 repeat all this for $Y$ and put everything together in equation (B.12).
References


[40] Lusseau D 2003 Proc. R. Soc. B 270 S186