Optimal map of the modular structure of complex networks

A Arenas\textsuperscript{1,2\dag}, J. Borge-Holthoefer\textsuperscript{1}, S Gómez\textsuperscript{1} and G Zamora\textsuperscript{3}

\textsuperscript{1} Departament d'Enginyeria Informàtica i Matemàtiques, Universitat Rovira i Virgili, 43007 Tarragona, Spain
\textsuperscript{2} Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA
\textsuperscript{3} Interdisciplinary Center for Dynamics of Complex System, University of Potsdam, 14415 Potsdam, Germany

E-mail: alexandre.arenas@urv.cat, javier.borge@urv.cat, sergio.gomez@urv.cat and gorka_agnld@yahoo.es

Abstract. Modular structure is pervasive in many complex networks of interactions observed in natural, social and technological sciences. Its study sheds light on the relation between the structure and function of complex systems. Generally speaking, modules are islands of highly connected nodes separated by a relatively small number of links. Every module can have contributions of links from any node in the network. The challenge is to disentangle these contributions to understand how the modular structure is built. The main problem is that the analysis of a certain partition into modules involves, in principle, as many data as number of modules times number of nodes. To confront this challenge, here we first define the contribution matrix, the mathematical object containing all the information about the partition of interest, and after, we use a Truncated Singular Value Decomposition to extract the best representation of this matrix in a plane. The analysis of this projection allow us to scrutinize the architecture of the modular structure, revealing the structure of individual modules and their interrelations.

\dag Author to whom any correspondence should be addressed
1. Introduction

The finding of modular structure in real complex networks [1] is revolutionizing the understanding of the evolution of complex systems [2]. Many efforts have been devoted to its automatic detection [3, 4, 5], however very little is known yet about the actual architecture of the detected modules that build the network. This architecture promises to be relevant to understand why physical processes in complex networks, such as synchronization [6], present emergent phenomena that are affected by the existence of topological barriers between modules. We still miss fundamental tools to anticipate these phenomena from a topological perspective. The current work is intended to provide network scientists with novel tools to screen the modular structure. The comprehension of modular structure in networks necessarily demands the analysis of the contribution of each one of its constituents (nodes) to the modules. Recently, Guimerà et al. [7, 8] advanced on this issue proposing two descriptors to characterize the modular structure: the $z$-score (a measure of the number of standard deviations a data point is from the mean of a data set) of the internal degree of each node in its module, and the participation coefficient ($P$) defined as how the node is positioned in its own module and with respect to other modules. Given a certain partition, the plot of nodes in the $z-P$ plane admit an heuristic tagging of nodes’ role. The success of this representation relies on a consistent interpretation of topological roles of nodes.

Here we introduce a formalism to reveal the characteristics of networks at the topological mesoscale, where the representation of the network is viewed as a set of interconnected modules. We propose a method, based on linear projection theory, to study the modular structure in networks that enables a systematic analysis and elucidation of its architecture. First, we construct a matrix containing all the information about the modular structure, and second, we find an optimal dimensional reduction of the information contained in it. In particular, we present the optimal mapping of the information of the modular structure (in the sense of least squares) in a two-dimensional space. The method has been applied to two empirical networks. The statistical analysis of the geometrical projections allow to characterize the structure of individual modules and their interrelations in a unified framework.

2. Projection of the modular structure

A complex network (weighted or unweighted, directed or undirected) can be represented by its adjacency matrix $A$, whose elements $A_{ij}$ are the weights of the connections from any node $i$ to any node $j$. Assuming that a certain partition of the network into modules is available, we plan to analyze this coarse grained structure. The main object of our analysis is the Contribution matrix $C$, of $N$ nodes to $M$ modules. The elements $C_{ia}$ are the number of links that node $i$ dedicates to module $a$, and can be easily obtained...
as the matrix multiplication between $A_{ij}$ and the partition matrix $S$:

$$C_{i\alpha} = \sum_{j=1}^{N} A_{ij} S_{j\alpha}$$

where $S_{j\alpha} = 1$ if node $j$ belongs to module $\alpha$, and $S_{j\alpha} = 0$ otherwise. The rows of $C$ correspond to nodes, and the columns to modules. The analysis of this matrix is the focus of our research. The goal is to reveal the structure of individual modules, and their interrelations. To this end, we propose to deal with the high dimensionality of the original data by constructing a two-dimensional map of the contribution matrix, minimizing the loss of information in the dimensional reduction, and making it more amenable to further investigation.

2.1. Singular Value Decomposition of the modular structure

The approach developed here consists in the analysis of $C$ using Singular Value Decomposition [9] (SVD). It stands for the factorization of a rectangular $N$-by-$M$ real (or complex) matrix as follows:

$$C = U \Sigma V^\dagger$$

where $U$ is an unitary $N$-by-$N$ matrix, $\Sigma$ is a diagonal $N$-by-$M$ matrix and $V^\dagger$ denotes the conjugate transpose of $V$, an $M$-by-$M$ unitary matrix. This decomposition corresponds to a rotation or reflection around the origin, a non-uniform scale represented by the singular values (diagonal elements of $\Sigma$) and (possibly) change in the number of dimensions, and finally again a rotation or reflection around the origin. This approach and its variants have been extraordinarily successful in many applications [9], in particular for the analysis of relationships between a set of documents and the words they contain. In this case, the decomposition yields information between word-word, word-document, and document-document semantic associations, the technique is known as Latent Semantic Indexing [10], and Latent Semantic Analysis [11]. Our scenario is quite similar to this, where nodes resemble words, and modules resemble documents. We devise that a similar approach will help to unravel the relations between nodes’ contributions and modules of a certain partition.

2.2. An optimal 2D map of the modular structure of networks

A practical use of SVD is dimensional reduction approximation (also known as Truncated Singular Value Decomposition, TSVD). It consists in keeping only some of the largest singular values to produce a least squares optimal, lower rank order approximation (see Appendix). In the following we will consider the best approximation of $C$ by a matrix of rank $r = 2$.

The main idea is to compute the projection of the contribution of nodes to a certain partition (rows of $C$, namely $n_i$ for the $i$-th node) into the space spanned by the first two right singular vectors, the projection space $U_2$ (see Appendix). We
denote the projected contribution of the \(i\)-th node as \(\tilde{n}_i\). Given that the transformation is information preserving [12], the map obtained gives an accurate representation of the main characteristics of the original data, visualizable and, in principle, easier to scrutinize. Note that the approach we propose has essential differences with classical pattern recognition techniques based on TSVD such as Principal Components Analysis (PCA) or, equivalently, Karhunen-Loeve expansions. Our data (columns of \(C\)) cannot be independently shifted to mean zero without losing its original meaning, this restriction prevents the straightforward application of the mentioned techniques, and also differentiate our work from the modern techniques for the analysis of gene expression patterns [13, 14].

The main problem when using SVD relies always on the interpretation of its outcome. The combination of data in the process makes difficult a direct comparison between input and output. To overcome this problem, we point out the following geometrical properties of the projection of the rows of \(C\) we have defined (see Appendix for a mathematical description):

(i) Every module \(\alpha\) has a distinguished direction \(\tilde{e}_\alpha\) in the projection space \(\mathcal{U}_2\) corresponding to the line of the projection of its internal nodes (those that have links exclusively inside the module), we call these directions intramodular projection;

(ii) Every module \(\alpha\) has an intrinsic direction \(\tilde{m}_\alpha\) in the projection space \(\mathcal{U}_2\) corresponding to the vector sum of the contributions of all its nodes, we call these directions modular projection;

(iii) Any node’ contribution projection \(\tilde{n}_i\) is a linear combination of intramodular projections, being the coefficient of each one proportional to the original contribution \(C_{i\alpha}\) of links of the node \(i\) to each module \(\alpha\).

Consequently, for those projections of nodes lying on the intramodular projection of its module, the distance to the origin is proportional to its degree (or strength). For those projections not lying on the direction of the intramodular projection of its module, the separation from this line provides information about the devotion of a node to connect with other modules. These geometrical facts are the key to relate the outcome of TSVD and the original data in our problem.

2.3. Structure of individual modules

To study the structure of individual modules we concentrate on the analysis of the projection of nodes’ contributions in the plane \(\mathcal{U}_2\). Keeping in mind the geometrical properties (1 and 3) exposed above, we propose to extract structural information relative to each module by comparing the map of nodes’ contributions to the intramodular projection directions. To this end it is convenient to change to polar coordinates, where for each node \(i\) the radius \(R_i\) measures the length of its contribution projection vector \(\tilde{n}_i\), and \(\theta_i\) the angle between \(\tilde{n}_i\) and the horizontal axis. We also define \(\phi_i\) as the absolute
distance in angle between $\vec{\mathbf{n}}_i$ and the intramodular projection $\vec{\mathbf{e}}_\alpha$ corresponding to its module $\alpha$, i.e. $\phi_i = |\theta_i - \theta_{\vec{\mathbf{e}}_\alpha}|$.

Using these coordinates $R-\phi$ we find a way to interpret correctly the map of the contribution matrix in $U_2$: i) $R_{\text{int}} = R \cos \phi$ informs about the internal contribution of nodes to its corresponding module, as well as to the contribution to its own module by connecting to others. To clarify the latter assertion, let us assume a node $i$ belonging to a module $\beta$ has connections with the rest of modules in the network. Given that this connectivity pattern is a linear combination of intramodular directions, the vector sum implies that connecting with modules $\alpha$ having $|\theta_{\vec{\mathbf{e}}_\beta} - \theta_{\vec{\mathbf{e}}_\alpha}| > \pi/2$ decreases the module $R$, and vice versa. ii) $R_{\text{ext}} = R \sin \phi$ informs about the deviation (as the orthogonal distance) of each node to the contribution to its own module.

We explore the internal structure of modules using the values of $R_{\text{int}}$, and the boundary structure of modules using $R_{\text{ext}}$. Using descriptive statistics one can reveal and compare the structure of individual modules. Provided that the distribution of contributions is not necessarily Gaussian, an exploration in terms of z-scores is not convenient. Instead we use box-and-whisker charts for the variables, depicting the principal quartiles and the outliers (defined as having a value more than 1.5 IQR lower than the first quartile or 1.5 IQR higher than the third quartile, where IQR is the Inter-Quartile Range).

The boxplots for the data of each module in the variable $R_{\text{int}}$ allow for a visualization of the heterogeneity in the contribution of nodes building their corresponding modules, and an objective determination of distinguished nodes on its structure (outliers). Consequently, the boxplots in $R_{\text{ext}}$ inform about the heterogeneity in the boundary connectivity. Nodes’ contribution projections that have $\phi = |\theta - \theta_{\vec{\mathbf{e}}_\alpha}| = 0$ (i.e. with links in only one module links) are not considered in this statistics because they do not provide relevant information about the boundaries, only nodes that act as bridges between modules are taken into account. Moreover, considering internal nodes in this statistics would eventually produce a collapse of the quartiles to zero. Assuming that every module devotes some effort to link the structure, the width of the boxes in this plot is proportional to the heterogeneity of such efforts, they inform about how well distributed is this effort among nodes. Furthermore, given two boxes equally wide, its position determines which module contributes the most to the connection of the whole network.

2.4. Interrelations between modules

The analysis of the interrelations between modules is performed at the coarse grained level of its modular projections. The modular projections $\vec{\mathbf{m}}_\alpha$ are aggregated measures of the nodes’ contribution to their particular module. The normalized scalar product of modular projections provide a measure of the interrelations (overlapping) between different modules. A representation of these data in form of a matrix ordered by the values of $\theta_{\vec{\mathbf{e}}_\alpha}$ reveals the actual architecture of the network at the topological mesoscale.
3. Application to real networks

The proposed mapping is applied here to two real networks, the worldwide air transportation network, and the AS–P2P Internet network. The airports network data set is composed of passenger flights operating in the time period November 1, 2000, to October 31, 2001 compiled by OAG Worldwide (Downers Grove, IL) and analyzed previously by Prof. Amaral’s group [8]. It consists of 3618 nodes (airports) and 14142 links, we used the weighted network in our analysis. Airports corresponding to a metropolitan area have been collapsed into one node in the original database. The AS–P2P Internet data set considered is composed of Autonomous Systems (AS) [15] in the peer to peer (P2P) category, where two ASs freely exchange traffic between themselves and their customers, but do not exchange traffic from or to their providers or other peers [16]. We complemented this data set with the geographic localization of the ASs, resulting in 1217 nodes and 4058 links. We have optimized modularity [3] to find good partitions of the networks in modules. We have used the partition corresponding to 26 modules and modularity $Q = 0.649$ for the airports network, and 12 modules and $Q = 0.387$ for the AS–P2P network, resulting from optimizing modularity with Extremal Optimization [17] and refined with Tabu search [18]. Note that any partition, not necessarily the one corresponding to optimal modularity, can be analyzed as described.

The interesting aspect of applying the analysis to these two data sets is twofold: first, since both are geo-referenced, it is possible to assign a tag to each module corresponding to geographic areas, and second, the modular structure of both networks is substantially different, while the airports network evolution has been mainly shaped by two well defined continental blocks (USA and W Europe)§, the AS–P2P network has been built in a fairly more homogeneous way. It is very interesting to observe how the AS–P2P network, following a sort of “wiring optimization”, presents a community structure evenly distributed in areas covering a worldwide belt.

In Fig. 1a,b, we plot the structure of the networks partitioned in modules, these conform the original data that compose our contribution matrices. The plots Fig. 1c,d (left) show the projections of the nodes’ contributions in the plane spanned by the two first right singular vectors $U_2$, as well as the intramodular projections of each module in this plane. The data in $U_2$ are transformed to polar coordinates for a better visualization and simpler analysis, see Fig. 1c,d (right). The differences between both modular structures has clearly emerged in this projection, the airports network is basically polarized in two geographical areas, whereas in the AS–P2P network this polarization does not exist. We also see how different airports and ASs excel in their values of $R$ largely over the rest. This effect can be further developed by studying the structure of modules and their interrelations in each case.

§ We denote N-S-E-W for the four cardinal points North, South, East and West respectively.
Figure 1. Optimal map of the modular structure for the optimal partition of the airports network (a) and the AS–P2P network (b), each color corresponds to a different module of the given partition. In (c) and (d) we plot the projected space spanned by the two left eigenvectors of the TSVD, $U_2$ (left), and its transformation to polar coordinates $R-\theta$ (right), for each network. Dashed lines mark the directions of intramodular projections of each module. Nodes whose contribution is totally internal to a module project exactly on its corresponding dashed line. In the $R-\theta$ plot we have labelled certain distinguished nodes that also correspond to very important airports and ASs in the world. The loss of information associated to the two-dimensional projection is 18.2% for the airports network and 15.8% for the AS–P2P network.
Figure 2. Box-and-whisker plots of $R_{\text{int}}$ and $R_{\text{ext}}$ respectively, for the two networks depicted in Fig 1. Modules are sorted according to medians in increasing order. We label the horizontal axis using names for the modules assigned according to the geographical location of at least the 75% of their nodes. We highlight whiskers and outliers in both networks.
The structure of modules is scrutinized in Fig. 2, where we depict the box-and-whisker plots of the internal contributions \( R_{\text{int}} \) and external contributions \( R_{\text{ext}} \). The results show the heterogeneity of each module of the partition. Remarkably, the method reveals outliers distinguished by its capability to support the internal structure of modules and also to cross-connect them. In Fig. 2a (top), we observe that USA and W Europe modules have medians greater than the percentiles-75 of the rest of modules. This fact is pointing out the extreme internal cohesion of both sites. We also observe that the lower in \( R_{\text{int}} \) median is Alaska, however Anchorage leads the internal cohesion orders of magnitude beyond the core. In Fig. 2a (bottom) Canada, W Europe an C America provide the highest profile of boundary connectivity. Nevertheless, the role played by USA is still very significant because of its high percentiles and outliers. On the other side, Africa, Russia and China are less connected to the world than the rest of modules. For the AS–P2P the box-and-whisker plots in \( R_{\text{int}} \) Fig. 2b (top) inform about a slight dominance of 3 modules E Europe (Germany, Austria, Italy and some others), W Europe (UK, the Netherlands, Belgium mainly) and the module containing USA and Japan. In \( R_{\text{ext}} \) Fig. 2b (bottom) the similarity in range and medians reveals the homogeneity of the mesoscale of this network. Significantly, some highlighted ASs in the plot do not belong geographically to the assigned tag, although the main proportion of nodes in that module do (see E Europe, W Europe and Russia).

Finally, the interrelations between modules is unveiled in Fig. 3 where it can be observed the different architecture of both networks. In the airports network a polarized structure of two continental blocks leaded by USA and Western Europe emerge, denoting the result of a long-standing history of aviation communication in both sites. In contrast, the AS–P2P Internet network presents a more intricate structure of several linchpins that support the whole AS–P2P worldwide connections. Specifically, we observe how the airports network structure is basically supported by the two main sites USA and W Europe, absorbing in its scope many other modules at each side of the Atlantic. However, three special modules emerge in the center of the matrix playing an special role in the whole structure, they correspond to Canada, C and S America and Japan that are essential connectors of both sites. Japan is still more interesting by no maintaining a preference in connections with both sites but with almost any module in the network. In the AS–P2P network we identify four groups, two of them big groups, one intermediate and an almost isolated group. The order of the labels of the plots (again, decreasing order of modular projection’s angle) show two interesting properties of this mesoscale: (i) from left to right (or top to bottom) the mesoscale comprises the Pacific Ocean block with the exception of South Africa, which is a satellite of USA in this mesoscale. Moving further, we found Canada at right and also South Korea representing half Pacific area. From right to left (bottom to top) we have E Europe, then W Europe and Europe-Asia-USA conforming the Atlantic block. Another step in the mesoscale and we find Russia. The only module still left is the blue one, corresponding mainly to Central Europe, although with ASs in Japan and USA, linking and completing the word-tour; and (ii) geographically misclassified ASs (see outliers in Fig. 2) confirm the roughly ring-shaped
Figure 3. Overlap matrices between the modules composing the topological mesoscale of the networks plotted in Fig. 1. Each matrix corresponds to the normalized scalar product of the individual modular projections (see text for details). Modules are sorted by decreasing order of modular projection’s angle in the plane $U_2$. 
structure of the mesoscale, where some modules are linked to the adjacent community via a geographically distant AS.

Summarizing, we have proposed a method based on Truncate Singular Value Decomposition to map the modular structure of complex networks in two-dimensions and found a set of geometrical relations to interpret this mapping. The effect of TSVD is to regularize the contributions of nodes to the modular structure, by reducing the complexity of the original data, minimizing the loss of information. Using this approach, the analysis of the structure of modules and their interrelations becomes easy and standardizable. We have presented the application to two real examples: the airport network and the AS–P2P internet network. While both networks are geo-referenced, our analysis captures the intrinsic structural differences between them.

The method proposed might be very useful for scholars in different disciplines that want access to an easy and tractable map of the empirical complex network data according to a biological, functional or topological partitions. We devise that the analysis of this map will be very helpful to anticipate the scope of dynamic emergent phenomena that depend on the structure and relations between modules. Spreading of viruses or synchronization processes are natural candidates to be analyzed considering the organization of the map. Further studies of the similarities between nodes’ contribution projections can also help to classify networks according to the role profiles of nodes [19] and/or modules.

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Appendix A. Properties of TSVD

Let us assume that we preserve only the $r$ largest singular values and neglect the remaining substituting their value by zero, then the reduced matrix $C_r = U \Sigma_r V^\dagger$ has several mathematical properties worth to mention: first, it minimizes the Frobenius norm ($\|A\|_F = \sqrt{\text{trace}(AA^\dagger)}$) of the difference $\|C - C_r\|_F$, that means that among all possible matrices of rank $r$, $C_r$ is the best approximation in a least squares sense; second, $C_r$ is also the best approximation in the sense of statistics, it maintains the most significant information portion of the original matrix [12]. The left and right singular
vectors (from matrices $U$ and $V$ respectively) capture invariant distributions of values of the contribution of nodes to the different modules. In particular the larger the singular value the more information represented by their corresponding left and right singular vectors. We have used the LAPACK-based implementation of SVD in MATLAB. We warn that some numerical implementations of SVD suffer from a sign indeterminacy, in particular the one provided by MATLAB is such that the first singular vectors from an all-positive matrix always have all-negative elements, whose sign obviously should be switched to positive [20].

Appendix B. Projection using TSVD of rank 2

In the case of a rank $r = 2$ approximation, the unicity of the two-ranked decomposition is ensured [9] if the ordered singular values $\sigma_i$ of the matrix $\Sigma$, satisfy $\sigma_1 > \sigma_2 > \sigma_3$. This dimensional reduction is particularly interesting to depict results in a two-dimensional plot for visualization purposes. In the new space there are two different sets of singular vectors: the left singular vectors (columns of matrix $U$), and the right singular vectors (rows of matrix $V^\dagger$). Given that we truncate at $r = 2$, we fix our analysis on the two first columns of $U$, we call this the projection space $\mathcal{U}_2$. The coordinates $\tilde{n}_i$ of the projection of the contributions $n_i$ of node $i$ are computed as follows:

$$\tilde{n}_i = \Sigma_2^{-1}V^\dagger n_i \quad (B.1)$$

Here $\Sigma_2^{-1}$ denotes the pseudo-inverse of the diagonal rectangular matrix $\Sigma_2$ (singular values matrix truncated in 2 rows), simply obtained by inverting the values of the diagonal elements. It is possible to assess the loss of information of this projection compared to the initial data by computing the relative difference between the Frobenius norms:

$$E_r = \frac{\|C\|_F - \|C_r\|_F}{\|C\|_F} = \frac{\sum_{\alpha=1}^{M} \sigma_\alpha^2 - \sum_{\alpha=1}^{r} \sigma_\alpha^2}{\sum_{\alpha=1}^{M} \sigma_\alpha^2} \quad (B.2)$$

Appendix C. Geometrical properties of the projection of $C$

The intramodular projection $\tilde{e}_\alpha$ corresponding to module $\alpha$, is defined as the projection of the cartesian unit vector $e_\alpha = (0, \ldots, 0, 1, 0, \ldots, 0)$ (the $\alpha$-th component is 1, the rest are zero), i.e.

$$\tilde{e}_\alpha = \Sigma_2^{-1}V^\dagger e_\alpha \quad (C.1)$$

Any node in the original contribution matrix can be represented as

$$n_i = \sum_{\alpha=1}^{M} C_{i\alpha} e_\alpha \quad (C.2)$$
Its projection gives the eigennode
\[ \tilde{n}_i = \sum_{\alpha=1}^{M} C_{i\alpha} (\Sigma_2^{-1} V^i e_\alpha) = \sum_{\alpha=1}^{M} C_{i\alpha} \tilde{e}_\alpha \]  
(C.3)
a linear combination of intramodular projections. In particular, a node \( i \) whose contribution is totally internal to a module \( \alpha \) is projected as \( \tilde{n}_i = k_i \tilde{e}_\alpha \), where \( k_i \) is the node degree. The modular projections \( \tilde{m}_\alpha \) are computed as the vector sum of all the projections of nodes contributions, for those nodes belonging to module \( \alpha \), i.e.
\[ \tilde{m}_\alpha = \sum_{i=1}^{N} S_{i\alpha} \tilde{n}_i \]  
(C.4)

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