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SPECTRAL TECHNIQUES IN COMPLEX NETWORKS

Abstract. Most physical, biological, chemical, technological and social systems have a network structure. Examples of complex networks range from cell biology to epidemiology or to the Internet. In the recent years, several models of complex networks have been proposed, as the random graph of Erdős and Rényi, the small-world model of Watts and Strogatz or the scale-free networks of Barabási and Albert.

The topological structure of such networks can be fully described by the associated adjacency matrices and their spectral density. The rich information about the topological structure and diffusion processes can be extracted from the spectral analysis of the networks. For instance, the power-law behavior of the density of eigenvalues is a notable feature of the spectrum of scale-free networks. Dynamical network processes, like synchronization can be determined by the study of their Laplacian eigenvalues. Furthermore, the eigenvalues are related to many basic topological invariants of networks such as diameter, mean distance, betweenness centrality, etc.

Spectral techniques are also used for the study of several network properties: community detection, bipartition, clustering, design of highly synchronizable networks, etc.

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1. Introduction

Complex networks are everywhere. They are formed by a large set of vertices representing the entities of the system, and a set of edges, representing the interactions between their elements. Examples of complex networks include the Internet, World Wide Web, social networks of acquaintances or other connections between individuals, distribution networks such as postal delivery routes, neural networks, food webs, metabolic networks, networks of citations between papers, organizational networks and networks of business relations between companies, and many others (see Fig. 1). In the recent last years, two classes of complex networks have aroused a great deal of interest in the literature: small-world networks and scale-free networks, as many real networks exhibit characteristics of both classes.

The spectrum of the adjacency and *Laplacian* matrices provide a great deal of information about the structure of a network. As usual, the eigenvalues of the adjacency matrix are denoted by λ_i , $1 \leq i \leq n$. Recall that the *Laplacian* matrix of a graph is a symmetric matrix L whose diagonal elements l_{ii} are the degrees of the vertices, and whose off-diagonal elements l_{ij} are -1 if the vertex v_i is connected to v_j , and 0 otherwise. More precisely, if D is the diagonal matrix of vertex degrees d_i and A is the adjacency matrix of the graph, $L = D - A$. Note that L is semi-positive definite, $x^T L x \geq 0$ for any vector x , its first eigenvector is $j = (1, \dots, 1)^T$ corresponding to the first eigenvalue $\theta_1 = 0$, and the second largest eigenvalue θ_2 is called the *algebraic connectivity* or *Fiedler value*, because its proximity to 0 reveals whether the graph can be easily disconnected. Its corresponding eigenvector v_2 is also known as the *Fiedler vector*, and is essential for the bisection method. The *Laplacian spectrum* is denoted by

$$\text{sp}(L) = \{0 \leq \theta_2 \leq \dots \leq \theta_n\}.$$

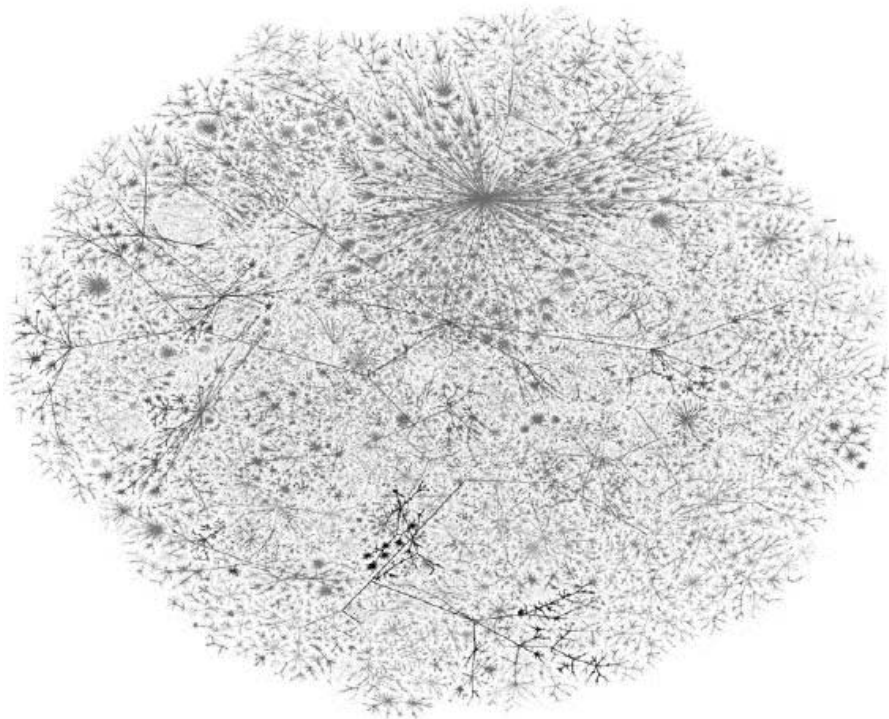


FIGURE 1. A complex network: a picture of the World Wide Web, from Hal Burch and Bill Cheswick, Lumeta Corp.

The *normalized Laplacian* matrix is introduced by Chung and defined as the symmetric matrix \mathcal{L} whose diagonal elements l_{ii} are 1, and whose off-diagonal elements $l_{ij} = -1/\sqrt{d_i d_j}$ if the vertex v_i is connected to v_j , and 0 otherwise. Its relation with the Laplacian is given by $\mathcal{L} = D^{-1/2} L D^{-1/2}$.

Several topological parameters are considered for the study of complex networks. Some of them are well known in graph theory, like the *diameter*, *mean distance*, *isoperimetric number*, *maximum and minimum degree* and *edge connectivity*.

The *edge connectivity*, $e(G)$, of a graph G is the minimum number of edges which must be deleted in G to disconnect it. The *minimum and maximum degree* of the graph are denoted by δ and Δ respectively. Denoting by $d(u, v)$ the distance between two vertices $u, v \in V(G)$ (the length of the shortest path), the *diameter* is $D = \max_{u, v \in V} d(u, v)$, and the *mean distance* or *average path length* is

$$\bar{l} = \frac{2}{n(n-1)} \sum_{(u,v) \in V(G)} d(u, v).$$

The graph diameter provides an inverse measure of the vertex connectivity. Intuitively, we can say that two vertices in a network are weakly connected if their

shortest connection passes through many other vertices. When this happens for all pairs of nodes, the diameter D of the graph is large.

The *isoperimetric number* of a graph is introduced by Mohar in [42] as the number $i(G) = \min_{|X| \leq \frac{n}{2}} |\delta X|/|X|$, where X is a subset of vertices, δX is the boundary of X , i.e., the set of edges in G between vertices in X and vertices not in X . It is a measure of whether or not a graph can be split in two subgraphs of the same cardinality. In the same paper there are two different bounds for the isoperimetric number.

New parameters and tools are also considered to characterize properties of these new networks, like the degree distribution, eigenvalue distribution, spectral density, clustering parameter and betweenness centrality.

Clustering parameter. Let e_i be the number of edges connecting the neighbors of a vertex u_i of degree δ_i , then the clustering coefficient of u_i is $C_i = 2e_i/\delta_i(\delta_i - 1)$, for any $1 \leq i \leq n$, and the clustering coefficient or parameter of the graph G is defined as

$$C = \frac{1}{n} \sum_{i=1}^n C_i.$$

Power-laws distributions. A power-law function follows the polynomial form $f(x) = ax^{-\gamma}$, where a, γ are constants and γ is called the power-law exponent. This kind of distribution was previously known as Pareto distribution or Zipf's law. The main property of power laws is their scale invariance, i.e., any scaling of the argument x by a constant factor causes only a proportionate scaling of the function itself, i.e., $f(cx) = a(cx)^{-\gamma} = c^{-\gamma}f(x) \propto f(x)$, which means that they are proportional and therefore it preserves the shape of the function itself. Moreover, by taking logarithms a linear relation is obtained $\log f(x) = \log a - \gamma \log x$. A network with degree power law distribution is called *scale-free*.

Spectral density. Given a graph G of order n , and adjacency matrix eigenvalues λ_i , $1 \leq i \leq n$, the spectral density of the graph is defined as

$$\rho(x) = \frac{1}{n} \sum_{j=1}^n \delta(x - \lambda_j), \quad \text{where } \delta(x) = \begin{cases} 1, & \text{if } x = 0, \\ 0, & \text{if } x \neq 0. \end{cases}$$

is the Kronecker or delta function.

Betweenness centrality. Vertex betweenness centrality was introduced by a sociologist Freeman [29] in 1977, as a measure of the importance of a vertex in a network. Since the appearance of complex networks it has become an important parameter to study networks features [45], generalizing the concept for edge betweenness centrality. Spectral bounds for either the vertex betweenness and edge betweenness of a graph are studied in [15], and more general properties can be found in [32]. The *maximum betweenness centrality*, B_{\max} , is also considered for studying several aspects of the network, as its synchronization capability (Section 3), or used for performance of bisection methods (Section 4).

To be more precise, if $\sigma_{uv}(w)$ denotes the number of shortest paths from vertex u to vertex v that go through w , and σ_{uv} is the total number of shortest paths from u to v , then $b_w(u, v) = \sigma_{uv}(w)/\sigma_{uv}$. The betweenness of a vertex w is

$B_w = \sum_{u,v \neq w} b_w(u,v)$. The betweenness centrality of a graph G of order n is

$$\bar{B} = \frac{1}{n} \sum_{u \in V} B_u,$$

and the maximum betweenness of the graph G is $B_{\max} = \max\{B_u \mid u \in V\}$. The mean betweenness \bar{B} is closely related with the mean distance \bar{l} of the graph as $\bar{B} = (n-1)(\bar{l}-1)$ [15]. The same parameters can be defined for edges, and the most used one is the maximum edge betweenness centrality, \mathcal{B}^E .

2. Internet graph models and their spectra

Traditionally networks have been described by either regular graphs or random models like the classical model of Erdős–Rényi [22]. The later consists of a graph on n vertices, $G(n,p)$, where the vertices are connected between them with probability p . In particular the distribution of the degree of any particular vertex v is binomial

$$P(d_v = k) = \binom{n}{k} p^k (1-p)^{n-k}.$$

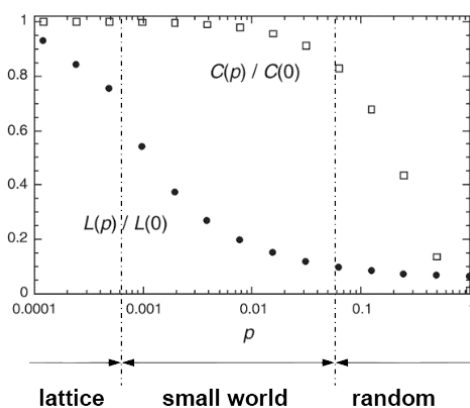


FIGURE 2. Watts and Strogatz small-world model. The diagram represents the rewiring probability p versus normalized mean distance \bar{l} and clustering parameter C . Observe that as p increases, both \bar{l} and C decrease. However, \bar{l} decays faster than C , which allows a probability region, $0.01 \leq p \leq 0.1$, where \bar{l} is a small and C is still high.

However, the appearance of new networks like the Internet graph, which could not be reproduced by these classical models, motivated Watts and Strogatz to introduce a new model for describing them [60]. They observed that such networks have a small diameter or mean distance as the former, and a large clustering parameter, as the later. Sparse random graphs have a small clustering coefficient while real world networks often have a coefficient significantly larger.

The model proposed by Watts and Strogatz starts from a regular graph with a large clustering parameter, which is transformed into a small world graph by the random reconnection of only a small number of edges, as the diameter is drastically reduced while the clustering coefficient of the regular graph remains large (see Fig. 2).

Since the appearance of this breakthrough a large number of stochastic and deterministic models have been appearing in the literature. For more information about them we refer the reader to the surveys [6] and [14].

In 1999 Faloutsos, Faloutsos and Faloutsos [25] made an experimental study of one part of the Internet graph, obtaining power laws in the distribution of many of the different parameters of the network, as the vertex degrees or the adjacency matrix eigenvalues. A typical value for the degree power-law exponent in real networks is $2 \leq \gamma \leq 3$. For obtaining the eigenvalue power-law, the eigenvalues λ_i of the adjacency matrix are sorted in decreasing order and plotted versus the associated increasing sequence of numbers i representing the order of the eigenvalue (see Fig. 3). A similar relation has been recently obtained for the normalized Laplacian eigenvalues in [53] and for the weighted Laplacian and the weighted adjacency matrix in [38]. Former experimental studies indicate that the power law exponents have not changed over the years in spite of the exponential network growth [34, 52].

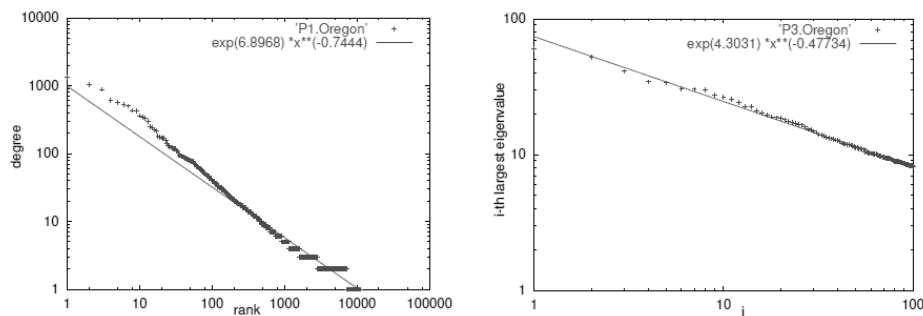


FIGURE 3. Power law distributions at the AS level Oregon Internet network, from [25]. On the left it is represented the histogram of 10000 highest vertex degrees and on the right the 100 largest eigenvalues versus their order, both in a log-log scale.

Mihail et al. in [41] found a surprising relationship between the degree and the eigenvalue exponents: the eigenvalue exponent is approximately half of the degree exponent. This fact indicates that the first largest eigenvalues are the square root of the first largest degrees. They also claimed that the eigenvalue distribution is a consequence of the degree distribution. However, in [31] it is proved by the construction of a deterministic model based on direct products of star graphs that the eigenvalue power-law is not a consequence of the degree power-law.

Among the scale-free models the most studied one is proposed by Barabási and Albert in 1999 [2]. The model is based on two observed facts in real networks: networks expand continuously by the addition of new vertices, and new vertices attach preferentially to sites that are already well connected. They used the so-called preferential attachment model. The model starts with a small number of vertices m_0 at step $t = 0$, and at every time step a new vertex u is connected to $m \leq m_0$ vertices of the existing graph. The probability of the new vertex u of being connected to an existing vertex u_i depends on its degree d_i , i.e.,

$$p(u \text{ is connected to } u_i) = p_i = \frac{d_i}{\sum_j d_j}, \text{ for } 1 \leq i \leq m.$$

The Barabási–Albert model produces a degree power-law distribution with exponent $\gamma = -3$, meanwhile the Watts and Strogatz and the Erdős–Rényi follow a Poisson distribution. This means that vertices with higher degree have stronger ability to grab links added to the network.

The main tool used for studying the spectra of large complex networks is the spectral density $\rho(\lambda)$. For a uncorrelated random graph, a graph where the probability for any pair of its vertices being connected is the same, p , and where these probabilities are independent variables, the adjacency matrix A is a real symmetric $n \times n$ uncorrelated random matrix, i.e., $EA_{ij} = 0$ and $EA_{ij}^2 = \sigma$. For this matrix, the limit of the spectral density when $n \rightarrow \infty$ converges to a semicircular distribution (if rescaled as $\lambda' = \lambda[np(1-p)]^{-1/2} \propto \lambda n^{-1/2}$)

$$\rho(\lambda') = \begin{cases} (2\pi)^{-1} \sqrt{4 - \lambda'^2}, & \text{if } |\lambda'| < 2, \\ 0, & \text{otherwise.} \end{cases}$$

This theorem is known as Wigner’s semicircular law [61]. Surprisingly, the semicircular spectral density is not valid for any realistic graph models.

The spectrum and the corresponding eigenvectors of the Barabási and Albert model have been studied by Goh et al. in [35] obtaining that the distribution of the spectra is quite far from a semicircle. The eigenvalues decay exponentially around the center and have power-law long tails at both edges. The same result was obtained by Farkas et al. in [26], where the spectral density of both Watts and Strogatz and Barabási and Albert models are studied, finding that they have a special shape. In particular, scale-free graphs develop a triangle-like spectral density with a power-law tail when plotted in log-log scale (see Fig. 4), while small-world graphs have a complex spectral density consisting of several sharp peaks (Fig. 5). They also found that the eigenvalues λ_1 and $|\lambda_n|$ depend on n as $n^{1/4}$ for large n , and that the eigenvector corresponding to the largest eigenvalue is strongly localized at the vertex with the largest degree and is independent of the system size n .

Nevertheless, Chung et al. [11] showed that, depending on the matrix, under a certain mild condition (that the minimum expected degree is significantly larger than the square root of the expected average degree), the eigenvalues of the normalized Laplacian of a random power-law graph follow the semicircle law, whereas the spectrum of the adjacency matrix of a power-law graph obeys the power law.

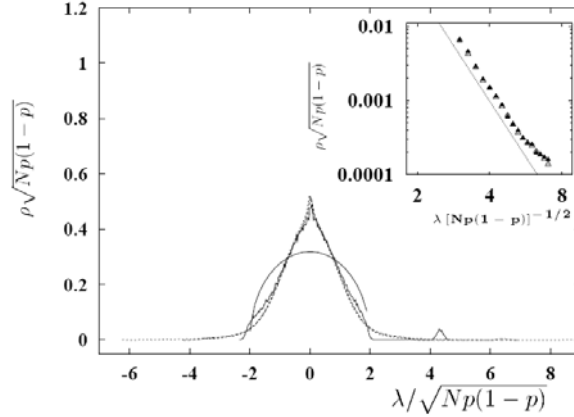


FIGURE 4. The spectral density of a Barabási-Albert graph with $m = 5$, and $n = 7000$ has a triangle-like shape compared with the semicircle, with a power-law decay in both sides. The isolated peak corresponds to the principal eigenvalue. In the upper corner the power-law decay is represented in a log-log scale. (from [26])

Furthermore, it has been reported that the k largest eigenvalues of the adjacency matrix of random power-law graphs have a power-law distribution (provided that the largest k degrees are large in the terms of the second-order average degree) [11, 26, 35, 41]. The k largest eigenvalues and eigenvectors have several applications in complex networks, as the search of clusters or communities (Section 4). For instance, Gkantsidis et al. [34] performed a comparison of clustering coefficients using the eigenvectors of the k largest eigenvalues of the adjacency matrices of Autonomous Systems (AS) topologies, where k is chosen to retain the strongest eigenvectors discarding most of the others. These and further results indicate that the spectra of correlated graphs represent a practical tool for graph classification and can provide useful insight into the relevant structural properties of real networks.

The spectra of the normalized Laplacian matrix of complex networks have been also studied, as it reflects global properties of the graph whereas the spectrum of the adjacency matrix contains information about local properties of the graph [11, 12]. Vukadinović et al. [57] were the first to investigate the properties of the AS topology based on the normalized Laplacian spectrum. They observed that it can be used to distinguish between synthetic topologies generated by graph generators like Inet and BGP. The eigenvectors corresponding to the largest eigenvalues of the Laplacian matrix can also be used to find clusters of AS with certain characteristics [34]

Other feature studied in [26] is the relation between the largest eigenvalue λ_1 and the "bulk" part of the spectrum $\lambda_2, \dots, \lambda_n$. It is shown that in the case

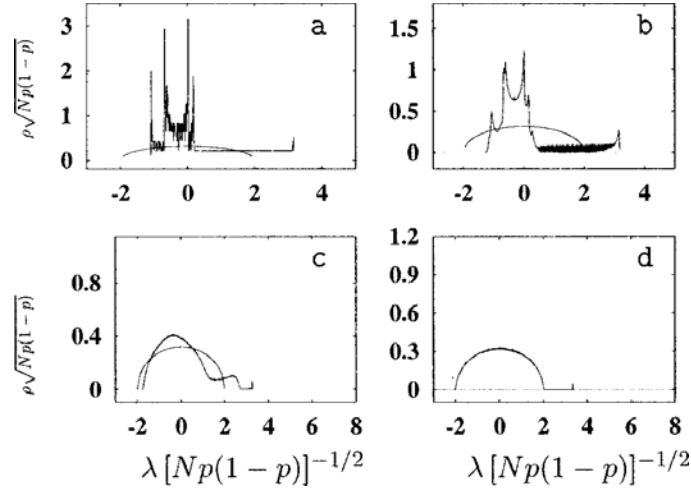


FIGURE 5. Spectral densities of several Watts and Strogatz small world models. The solid line shows the semicircular distribution for comparison: (a) with $p = 0$, $k = 10$ and $n = 1000$, the regular ring density is composed by a great deal of singularities, (b) with $p = 0.01$ the small-world graph density still has important singularities, (c) with $p = 0.3$ the small-world graph density is different from the semicircle shape, (d) and finally with $p = 1$ the uncorrelated random graph density has the semicircle shape. (from [26])

of random networks the largest adjacency eigenvalue grows much faster than the second largest one: $\lim_{n \rightarrow \infty} (\lambda_1/n) = p$ with probability 1, while for any $\epsilon > 1/2$, $\lim_{n \rightarrow \infty} (\lambda_2/n^\epsilon) = 0$. A similar relation holds for the smallest eigenvalue as well. This means that the spectral gap $g(A) = \lambda_1 - \lambda_2$ grows very fast, while the bulk of the spectrum is concentrated in a semi-circle denoted by $w(A) = \lambda_2 - \lambda_n$ (see Fig. 4). Similar situations have been observed for small-world graphs as well as for scale-free graphs. The bulk part of the scale-free graphs the spectral density is triangle-like instead of semi-circular in the scale-free case. For this reason, the quantity $R = (\lambda_1 - \lambda_2)/(\lambda_2 - \lambda_n)$ has been proposed as a measure of the distance of the first eigenvalue from the main part of the distribution of eigenvalues normalized by the extension of the main part (see Fig. 6). This ratio is intimate-related to some dynamical properties of the graph, as its synchronizability (Section 3).

Finally, the second largest eigenvalue of the Laplacian matrix or algebraic connectivity, has been also studied for either the Watts and Strogatz small-world model and the Barabási and Albert scale-free model in [58, 59]. For the former, they find a linear dependency between $-\theta_2$ and the rewiring probability p for a fixed n , that is, for any given value of n , $-\theta_2$ decreases to $-n$ as p increases from 0 to 1. And for the later they find that for any given value of $p \in (0, 1]$, $-\theta_2$ decreases to $-\infty$ as n increases to $+\infty$ (see Fig. 7 and Fig. 8)

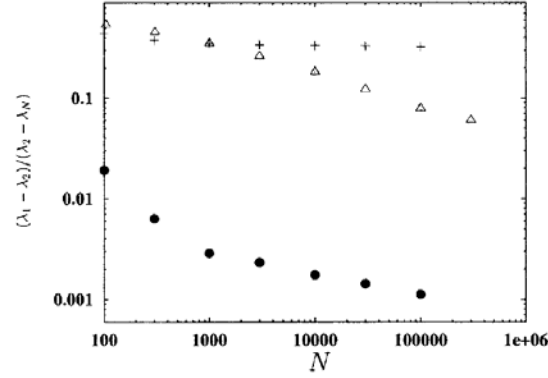


FIGURE 6. The ratio $R = (\lambda_1 - \lambda_2)/(\lambda_2 - \lambda_n)$ for a sparse uncorrelated random graph (+), small-world graph with $p = 0.01$ (•) and scale-free network (\triangle), versus the size of the graph n . Observe that for the first R converges to a constant, whereas for the others decays rapidly as $n \rightarrow \infty$. (from [26])

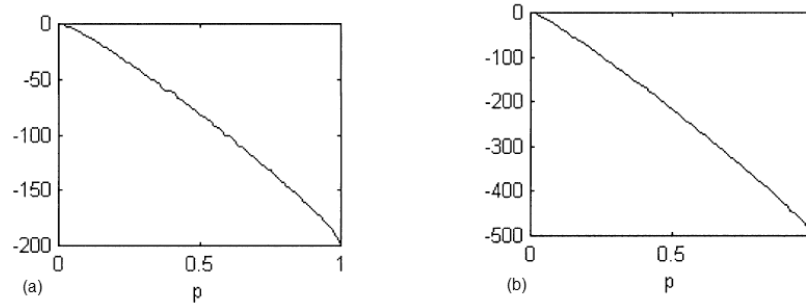


FIGURE 7. The opposite of the algebraic connectivity, $-\theta_2$, at two Watts and Strogatz models as a function of the probability, for (a) $n = 200$ and (b) $n = 500$. (from [59])

The opposite of the algebraic connectivity at the Barabási and Albert model is studied in [58] for three cases, obtaining in all of them that $-\theta_2$ bounded function as n increases to ∞ (Fig. 9). Observe that it has a small value, which implies that scale-free networks have poor synchronizability (Section 3).

3. Synchronization

Synchronization is the process where two or more systems interact with each other and come to move together. Synchronization processes are ubiquitous in nature and are present in many different contexts such as biology, technology, sociology, climatology, etc. The dynamics e.g., of the human cardiorespiratory system, of

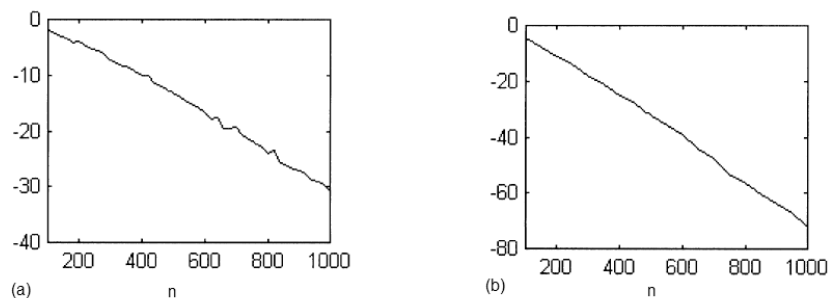


FIGURE 8. The opposite of the algebraic connectivity, $-\theta_2$, at two Watts and Strogatz models as a function of the size of the network n , for (a) $p = 0.05$ and (b) $p = 0.1$. (from [59])

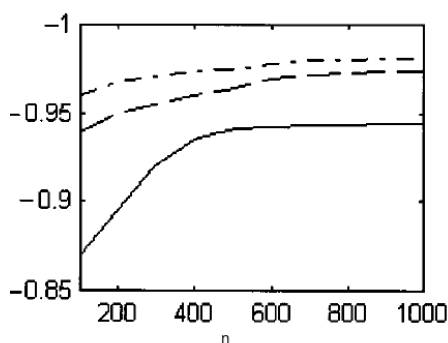


FIGURE 9. The opposite of the algebraic connectivity, $-\theta_2$, at the Barabási and Albert model with $m_0 = m = 3$ (lower), $m_0 = m = 5$ (middle) and $m_0 = m = 7$ (upper). (from [58])

an extended ecological system, of the magnetoencephalographic activity of Parkinsonian patients, and of electrosensitive cells of the paddlefish, have been shown to display synchronization features.

Historically, in 1667 Huygens observed the first synchronization phenomenon between two pendulum metronomes: putting them side by side oscillating at the same frequency with a 180° out of phase, after a small perturbation the clocks ended up synchronizing and persisted indefinitely. The synchronization of a few interacting oscillators has been widely studied in physics and mathematics literature, and also other aspects like the stability of the synchronization state against small perturbations. Initially, the attention was mainly focused to synchronization of periodic systems, while recently the interest for synchronization has moved to chaotic systems, as they are bound to be more common in nature. A dynamical system is called chaotic whenever its evolution sensitively depends on the initial

conditions. There are several types of synchronization features in chaotic systems: complete synchronization, lag synchronization, generalized synchronization, phase and imperfect phase synchronization. The most studied is the complete synchronization, which consists of the perfect hooking of the trajectories of a system of identical chaotic oscillators in the course of the time.

From different theoretical frameworks considered to study the synchronization of complex networks, their topology has turned out to play a crucial role in determining their dynamical behavior. Several models for real networks associated with complex systems are used to study relationships between the system synchronization and graph invariants, as well as some of the system relevant topological parameters. To be more precise, the Laplacian spectra and the algebraic connectivity or second smallest eigenvalue of the Laplacian matrix are important factors for obtaining the synchronization state or the stability of the synchronization state for some of these theoretical models. Their relation with other topological parameters of the network, as the diameter or the mean distance, provides some interesting conditions for existence of the synchronization. Besides, the recent appearance of large complex networks and the study of their dynamical characteristics, has become a new challenge for the scientific community. Synchronization in small-world and scale-free networks have aroused a great deal of interest. For more information about synchronization theory in dynamical systems we refer the reader to review papers [1, 5].

Therefore in this section we first study two of these theoretical frameworks relating synchronization with Laplacian eigenvalues. By using known bounds for the algebraic connectivity θ_2 and the largest Laplacian eigenvalue θ_n we derive bounds for the synchronization ratio θ_n/θ_2 . And finally we take advantage of the classical techniques from the spectral graph theory [17] to construct a large family of highly synchronizable networks.

Coupled identical oscillators. In the work [50] of Pecora and Carroll the stability of the synchronized state of a network of coupled identical oscillators is studied by using the so-called Master Stability Function. When all the oscillators are initially synchronized it is a crucial question to know whether this state is stable in the presence of small perturbations. The motion of a system is described by the general equation

$$\dot{x} = F(x), \quad x \in \mathbb{R}^n.$$

Considering linear time-continuous systems, this equation turns out into:

$$(3.1) \quad \dot{x}_i(t) = F(x_i(t)) + \sigma \sum_{j=1}^n L_{ij} H(x_j(t)), \quad i = 1, \dots, n,$$

where $x_i(t) = (x_{i_1}(t), \dots, x_{i_n}(t))^T \in \mathbb{R}^n$ represents the state variables at each oscillator i . The first part of the equation, $\dot{x}(t) = F(x(t))$ explains the dynamics of each node, and the function $H(x(t))$ is the output function (the same at each node), which represents the influence of network in the oscillator i . The parameter σ is the coupling strength, and L is the Laplacian matrix. There is a completely

synchronized state if

$$x_1(t) = x_2(t) = \dots = x_n(t) = s(t),$$

where $s(t)$ is the desired synchronized state. When all the oscillators are initially synchronized, they remain synchronized until the presence of small perturbation interferes. Now the question is whether the synchronization state is stable in the presence of small perturbations δx_i . In this case $x_i(t) = s(t) + \delta x_i$, and expanding the functions F and H to first order in a Taylor series, i.e., $F(x_i) = F(s) + DF(s)\delta x_i$ and $H(x_i) = H(s) + DH(s)\delta x_i$, where $DF(s)$ and $DH(s)$ are the Jacobian matrices of L and H on s respectively, we obtain the following variational linear equations for δx_i

$$\delta x_i = DF(s) + \sigma DH(s) \sum_{j=1}^n L_{ij} \delta x_j, \quad i = 1, \dots, n.$$

By projecting $\delta f x_i$ into the eigenspaces spanned by the eigenvectors v_i of the Laplacian matrix L , the former equations that can be diagonalized into blocks as

$$\dot{y}(t) = [DF(s) + \theta DH(s)]y(t),$$

where y represents the different perturbation modes from the synchronized state, $\theta = \sigma \theta_i$ for each i -block, with θ_i the i -th eigenvalue of the Laplacian matrix, $i = 1, \dots, n$. The idea is to project δx_i into the eigenspace spanned by the eigenvectors v_i of the coupling matrix L .

The linear stability of the synchronized state for any linear coupling is provided by the largest Lyapunov exponent of this equation $\Delta(\theta)$. In [50] it is shown that the synchronization state is stable if $\Delta(\sigma \theta_i) < 0$ for $i = 2, \dots, n$. Moreover, it has been found [3] that for many chaotic oscillators there exists a range of values in the interval (α_1, α_2) where this condition is satisfied. In this case, there exists a value of the coupling strength σ such that the synchronization state is linearly stable if and only if

$$\theta_n / \theta_2 < \alpha_2 / \alpha_1 \equiv \beta,$$

where β is a constant independent of the Laplacian matrix L . The values for β depend on the different kind of oscillator, but for many chaotic oscillators they use to be between 5 and 100 [50]. Therefore, for large values of θ_n / θ_2 it is not possible to obtain synchronization, independently of the value of the coupling strength and the kind of oscillator.

Furthermore, Wang and Chen in a former paper [58], study the asymptotical synchronization of a dynamical network model characterized by Equation 3.1 with $H(x_j(t)) = -x_j(t)$. It is said that the dynamical system reaches a state of asymptotical synchronization if

$$x_1(t) = \dots = x_n(t) = s(t),$$

when $t \rightarrow \infty$, where $s(t)$ can be an equilibrium point, a periodic orbit, or a chaotic attractor. They show that the system is exponentially stable if $1/\theta_2$ is bounded by a constant.

In both models we can see that the synchronization of the network depends on algebraic connectivity θ_2 . When it is close to 0, $1/\theta_2$ is large, then the network

cannot reach a synchronization state. Besides, in the first model the largest Laplacian eigenvalue θ_n has also a great influence, and more precisely the ratio θ_n/θ_2 , should also be small to attain synchronizability. Nevertheless, these two Laplacian eigenvalues by themselves do not provide information about the relationship between the network topology and the dynamics of synchronization. In the following subsection we will study some spectral bounds obtained from the classical spectral graph theory that will provide a connection between the synchronization of a network and several of its main invariants and parameters.

3.1. Synchronization and topological parameters. In order to characterize the synchronization of a network, we study the relationship between the inverse of the second eigenvalue of the Laplacian matrix, $1/\theta_2$, and the ratio θ_n/θ_2 , with other graph topological parameters like the minimum and maximum degrees, diameter, mean distance, isoperimetric number, betweenness centrality and clustering parameter. Most of these bounds can be found in [16]. From the bounds that can be obtained for $1/\theta_2$ and by using the classical bound $\Delta < \theta_n \leq 2\Delta$ provided by Fiedler [27] we can derive new lower and upper bounds for the synchronization ratio θ_n/θ_2 .

Minimum and maximum degrees of the graph. The minimum degree of a graph, δ , is related to the minimum connectivity of the graph. As $\theta_2 \leq \delta n/(n-1)$, and $\theta_n \geq (\Delta+1)$ (see [36]), one can obtain

$$\left(1 - \frac{1}{n}\right) \frac{(\Delta+1)}{\delta} \leq \frac{\theta_n}{\theta_2}.$$

When the difference between the maximum and minimum degree is large (heterogeneity), the synchronizability will be not reached. Now considering scale-free networks, for which $\delta = 1$, and Δ, n are large then $1 - 1/n \simeq 1$, and $(\Delta+1) \leq \theta_n/\theta_2$, which means that the network has a very low synchronization capability.

Edge connectivity. From a bound in [27] it can be easily obtained:

$$\frac{\theta_n}{\theta_2} \leq \frac{\Delta}{e(G)(1 - \cos \frac{\pi}{n})}.$$

Observe that when n is large the bound becomes independent of the value of $e(G)$, which does not provide much information.

Diameter. One of the bounds relating the algebraic connectivity with the diameter was given by Mohar in [43] as $D \geq 4/(n\theta_2)$ and so we obtain:

$$\frac{\theta_n}{\theta_2} \leq \frac{nD\Delta}{2}.$$

For graphs with a large D or n , this equation provides a large upper bound. However, if both values are small then the network will be easy to synchronize. A lower bound for the inverse algebraic connectivity can be obtained from the diameter bound $D \leq 2 \lceil \frac{\Delta+\theta_2}{4\theta_2} \ln(n-1) \rceil$ from [43], where Δ is the maximum degree of the graph:

$$\left(\frac{4}{\ln(n-1)} \lceil \frac{D}{2} \rceil - 1\right) \frac{(\Delta+1)}{\Delta} \leq \frac{\theta_n}{\theta_2}.$$

From the former equation, note that if $D \gg \ln(n-1)$, then the bound is greater than 1, and it will be difficult to reach a synchronization state provided that the maximum degree Δ is very large.

Now, consider the following bound in [43]: if there are two subsets of vertices, B and C , at distance $r+1$:

$$4(r-1)^2 \frac{|B||C|}{(n-|B|-|C|) \cdot (|B|+|C|)} < \frac{\theta_n}{\theta_2},$$

where $|B|$ and $|C|$ are the cardinalities of the subsets. If both subsets have only one vertex and they are at maximum distance D , the bound results

$$\frac{2(D-2)^2}{(n-2)} < \frac{\theta_n}{\theta_2}.$$

For large n and a small D the bound will tend to 0 and synchronization is possible. Also, for graphs with a diameter close to n would lead to large lower bound and the networks will not synchronize.

Studies about the diameter in small-world networks show that many real networks associated with complex systems have a logarithmic diameter $D \sim \ln n$ (similar to). In this case, the lower bound can be written approximately as $1/\Delta \leq 1/\theta_2$. Since the maximum degree Δ is also large, in scale-free networks the lower bound will approach 0 and synchronization is possible.

Mean distance. In [43] several bounds relating the mean distance with the algebraic connectivity can be found. Firstly we find this bound relating the mean distance with Q :

$$\bar{l} < \frac{n}{n-1} \left[1 + \sqrt{\frac{\theta_n}{\theta_2}} \sqrt{\frac{\alpha^2 - 1}{4\alpha}} \right] \left(\frac{1}{2} + \left\lceil \log_\alpha \frac{n}{2} \right\rceil \right),$$

where $\alpha > 1$ is a parameter. A large mean distance hinders the network synchronization. A lower bound can be obtained from

$$\bar{l} \leq \frac{n}{n-1} \left(\left\lceil \frac{\Delta + \theta_2}{4\theta_2} \ln(n-1) \right\rceil + \frac{1}{2} \right),$$

$$\left(\left\lfloor \frac{2\bar{l}(n-1) - n}{2n \ln(n-1)} \right\rfloor - \frac{1}{4} \right) \frac{4(\Delta + 1)}{\Delta} \leq \frac{\theta_n}{\theta_2}.$$

Note that as n becomes large, the bound takes a lower value if the mean distance is also small. However, if n is small and \bar{l} relatively large, the bound is also large and the synchronization of the network would not be possible. The maximum degree also is an influence on the synchronization, larger degrees make it easier.

Isoperimetric number of a graph or Cheeger constant. In [42] we find two different bounds for the isoperimetric number. The lower bound $i(G) \geq \theta_2/2$, gives us

$$\frac{\Delta + 1}{2i(G)} \leq \frac{\theta_n}{\theta_2}.$$

From this bound, if the isoperimetric number is near 0, the network will be easy to disconnect in two parts and by using the previous bound the inverse algebraic connectivity will be large, and the synchronization would not be possible. Cheeger

inequalities relate the isoperimetric number of a graph with its algebraic connectivity θ_2 and its maximum degree Δ . From the upper bound $i(G) \leq \sqrt{\theta_2(2\Delta - \theta_2)}$, we have the inequality $\theta_2^2 - 2\Delta\theta_2 + i(G)^2 \leq 0$ which leads us to

$$\frac{2}{1 + \sqrt{1 - (i(G)/\Delta)^2}} \leq \frac{\theta_n}{\theta_2} \leq \frac{2}{1 - \sqrt{1 - (i(G)/\Delta)^2}}.$$

In this case, if $i(G) \sim \Delta$, then both bounds in reach 2 and the synchronization should be possible, meanwhile if $i(G) \sim 0$ the lower bound goes to infinity and the network cannot synchronize.

Betweenness centrality and maximum betweenness centrality. The maximum betweenness centrality, B_{\max} , is larger than \bar{B} , so the corresponding lower bounds can also be used to obtain lower bounds. Moreover, in [15] a bound can be found that relates B_{\max} to the isoperimetric number:

$$B_{\max} + 2 \geq \frac{n}{\sqrt{\theta_2(2\Delta - \theta_2)}}.$$

Therefore it can be easily deduced that

$$\frac{\Delta}{\Delta + \sqrt{\Delta^2 - (n/(B_{\max} + 2))^2}} \leq \frac{\theta_n}{\theta_2} \leq \frac{2\Delta}{\Delta - \sqrt{\Delta^2 - (n/(B_{\max} + 2))^2}}.$$

Observe that if $(B_{\max} + 2)/\Delta \sim n$, then $\theta_n/\theta_2 \leq 2$ and synchronization is possible, but if $B_{\max} + 2 \sim 2n(n-1) + 2$ (as in a star graph), then $1/2\Delta \leq 1/\theta_2 \leq \infty$ and the bounds are not useful to describe the synchronizability of a network.

The following lower and upper bounds are given in [49]:

$$\left(1 - \frac{1}{n}\right) \frac{\Delta}{\delta} \leq \frac{\theta_n}{\theta_2} \leq (n-1)\Delta \mathcal{B}_{\max}^E D\bar{l},$$

where \mathcal{B}_{\max}^E is the maximum edge betweenness of the network [15, 33]. From the lower bound it can be deduced that the heterogeneity of degrees affects the synchronization of the network. A large difference between the maximum and minimum degrees makes the network more difficult to synchronize, which uses to happen in scale-free networks. However, homogeneous networks not always synchronize. Several studies on model networks corroborate this result in [30].

3.2. Design of synchronizable networks. As seen in previous sections, both scale-free and small-world networks display better synchronization than regular graphs [3]. However, it has also been observed that networks with strong heterogeneity in the degree distribution are much more difficult to synchronize than random homogeneous networks [49]. Donetti et al. in [19, 20] proposed entangled networks, which are extremely homogeneous regular networks, as examples of highly synchronizable networks. These graphs are obtained by using a numerical optimization algorithm, which excludes the possibility of using mathematical tools to generate infinitely many such networks. However, Estrada et al. [24, 7] propose a different approach, introducing a family of graphs (golden spectral graphs) which can be built by using analytical tools from the classical algebraic graph theory [17].

Observe that for a regular graph the synchronization ratio is related with R by

$$Q = \frac{\theta_n}{\theta_2} = \frac{\lambda_1 - \lambda_n}{\lambda_1 - \lambda_2} = \frac{\lambda_2 - \lambda_n}{\lambda_1 - \lambda_2} \cdot \frac{\lambda_1 - \lambda_n}{\lambda_2 - \lambda_n} = \omega_1(G) \cdot \omega_2(G) = \frac{1}{R} \cdot (R + 1),$$

where

$$\omega_1(G) = \frac{\lambda_2 - \lambda_n}{\lambda_1 - \lambda_2}, \quad \lambda_1 \neq \lambda_2, \quad \omega_2(G) = \frac{\lambda_1 - \lambda_n}{\lambda_2 - \lambda_n}, \quad \lambda_2 \neq \lambda_n,$$

are inverse, and therefore it is not easy to find graphs in which their product is small. This fact clearly hampers the synchronization of the network. In the search of graphs with small $Q = \omega_1(G) \cdot \omega_2(G)$, we consider those where both spectral ratios are equal, as it is straightforward to check that in this case $\omega_1(G) = \omega_2(G) = \varphi = (1 + \sqrt{5})/2$ and thus $Q = \varphi^2 = \varphi + 1$.

Definition 3.1. A golden spectral graph (GSG) is a graph for which both spectral ratios are identical, that is

$$\omega_1(G) = \omega_2(G) = \varphi,$$

where $\varphi = (1 + \sqrt{5})/2$ is the golden section, golden mean or divine proportion.

The first examples and properties of golden spectral graphs are found by Estrada in [7] and amplified in [24] by using classical spectral techniques, finding infinite families of such graphs (see Fig. 10).

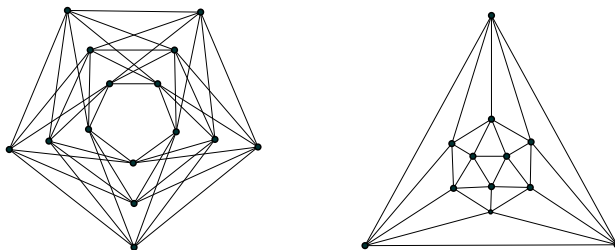


FIGURE 10. Two examples of highly synchronizable networks: $C_5 \otimes J_3$ and the icosahedral graph.

4. Community detection and spectral bisection

Empirical studies reveal a common property between many networks: community structure, i.e., the division of network vertices into groups with dense connections between them and sparse connections between groups [33, 47]. Communities are important because they often correspond to functional units such as cycles or pathways in metabolic networks or collections of pages on a single topic on the web. Moreover, networks can have properties at the community level that are quite different for the entire network.

A huge variety of community detection techniques have been developed, based on centrality measures, spectral techniques, flow models, random walks, resistor networks, optimization and many other approaches [18, 47]. There is a large literature about finding connections between divisions of networks and matrix spectra, the so-called spectral partition or spectral clustering [56]. The main tools for spectral clustering are graph Laplacian matrices or normalized Laplacian matrices. Most approaches to graph partitioning are based on iterative bisection methods, that is, finding the best division of the graph into two groups and then further subdividing those two into more groups. The spectral bisection method is originally due to Fiedler [27] and popularized by Pothen et al. [51], and is based on the Laplacian matrix eigenvectors. We describe here the simplest form of this method.

For dividing the graph into two subgraphs it is usual to consider the following parameter:

Definition 4.1. Given two subsets A and B of the vertex set $V(G)$ of a graph G and forming a partition of it, the number of edges connecting them is called the cut size

$$(4.1) \quad R = \frac{1}{2} \sum_{i \in A, j \in B} a_{i,j},$$

where the factor $1/2$ compensates for counting each edge twice.

Now consider an index vector s with n elements as

$$(4.2) \quad s_i = \begin{cases} 1, & \text{if } i \in A, \\ -1, & \text{if } i \in B. \end{cases}$$

Observe that $s^T s = n$, and

$$\frac{1}{2}(1 - s_i s_j) = \begin{cases} 1, & \text{if } i \text{ and } j \text{ are in different groups,} \\ 0, & \text{if } i \text{ and } j \text{ are in the same group.} \end{cases}$$

This allows us to rewrite Equation 4.1 as

$$R = \frac{1}{4} \sum_{i,j \in V(G)} (1 - s_i s_j) a_{i,j}.$$

Recalling that the degree of a vertex i is $k_i = \sum_j a_{ij}$, then

$$\sum_{i,j \in V(G)} a_{ij} = \sum_{i \in V(G)} k_i = \sum_{i \in V(G)} s_i^2 k_i = \sum_{i,j \in V(G)} s_i s_j k_i \delta_{ij},$$

where $\delta_{ij} = 1$ if $i = j$ and 0 otherwise. Therefore

$$R = \frac{1}{4} \sum_{i,j \in V(G)} s_i s_j (k_i \delta_{ij} - a_{i,j}) = \frac{1}{4} s^T L s.$$

Considering an orthogonal basis of Laplacian eigenvectors v_i , for $1 \leq i \leq n$, the index vector s can be expressed as a linear combination of the Laplacian eigenvectors,

$s = \sum_{i=1}^n \alpha_i v_i$, where $\alpha_i = v_i^T s$. Note that $\sum_{i=1}^n \alpha_i^2 = n$, then

$$R = \left(\sum_{i \in V(G)} \alpha_i v_i^T \right) L \left(\sum_{i \in V(G)} \alpha_i v_i \right) = \sum_{i \in V(G)} \alpha_i^2 \theta_i.$$

Therefore minimizing R implies minimizing α_i^2 . So fixing both sizes of the subgraphs $|A| = n_1$ and $|B| = n_2$, observe that $\alpha_1^2 = (v_1^T s)^2 = (n_1 - n_2)^2/n$. As we cannot vary this coefficient, R would be minimized by taking s proportional to v_2 (the Fiedler vector, which is orthogonal to v_i , for $i \geq 3$). However, the restriction due to Equation 4.2 implies that this cannot be possible in most of the cases, but a good approximation could be taking s as close to a parallel vector with v_2 as possible. This implies maximizing the quantity

$$|v_2^T s| = \left| \sum_{i=1}^n v_i^{(2)} s_i \right| \leq \sum_{i=1}^n |v_i^{(2)}|,$$

where $v_i^{(2)}$ are the i -components of the Fiedler vector. The maximum of $|v_2^T s|$ is reached when $v_i^{(2)} s_i \geq 0$ for all $1 \leq i \leq n$, that means that s_i must have the same sign as $v_i^{(2)}$. Therefore, the sign of each component $v_i^{(2)}$ of the Fiedler vector determines if the vertex i belongs to either A or B , which very often is against the condition of the desired sizes of the two subgraphs. In such a case, several options can be taken, as assigning either the most positive elements of s to the smaller group or to the larger group, and then taking the option which gives the smallest R .

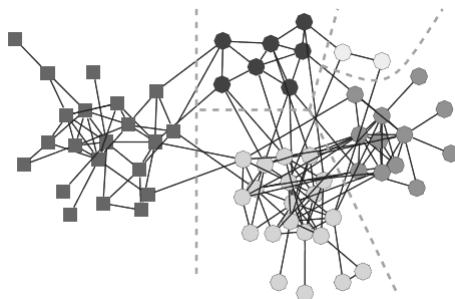


FIGURE 11. Community structure in the social network of bottlenose dolphins assembled by Lusseau et al. extracted using the algorithm of Girvan and Newman. The squares and circles denote the initial split of the network by using the bisection method. (from [47])

Consequently, the method does not guarantee to minimize R , but in many cases (when θ_2 is well separated from the rest of the eigenvalues), it does it very well. Generalizations of this method for a partition of k vertices subsets has been also

studied, and besides using other kinds of Laplacian matrices. For an extensive study about this subject we refer the reader to [56].

However, the method is a poor tool for detecting natural community structure in real-world networks, as the sizes of the groups are fixed from the beginning. Several approaches have been proposed to solve this problem. For this reason, Girvan and Newman [33] implemented an algorithm for calculating the modularity of the network, a new measure of how good is a particular division of the network is (see Fig. 11). That is, for a division with k groups, consider the $k \times k$ matrix E whose component e_{ij} is the fraction of edges in the original network that connect vertices in group i to those in group j . Then the modularity index is defined as

$$Q = \sum_i e_{ii} - \sum_{ijk} e_{ij}e_{ki}.$$

Physically Q is the fraction of all edges that lie within communities minus the expected value of the same quantity in a graph in which the vertices have the same degrees but where edges are placed at random without regard for the communities. If $Q = 0$ the community structure is not stronger than the one that can be expected by random chance. Local peaks in the modularity during the progress of the community structure algorithm indicate particularly good divisions of the network.

Modularity can also be approached by spectral methods. In [48] three spectral techniques can be found for approximating this parameter: the leading eigenvector method, other eigenvectors of the modularity matrix and a vector partitioning algorithm. All of them follow similar spectral techniques to the ones used in the first part of this section.

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