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On the second largest eigenvalue of networks

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Abstract

From predicting the epidemic threshold of a disease outbreak to anticipating the stability of a complex system, analysis of spectra of the adjacency matrices of the underlying networks play a pivotal role. Despite spectra of networks considered as fingerprints of the corresponding complex systems, most works and review articles have circumscribed around the largest eigenvalue (λ_1) only. The second largest eigenvalue of a network that admits many applications in diverse fields, including mathematics and computer science, has not been thoroughly contemplated. This article first reviews existing literature on λ_2, predominantly confined to the random regular graphs, followed by the results for various popular model networks. We emphasize the aspect that λ_2 shows an entirely different behavior than λ_1.

Keywords: Networks, Spectra

Introduction

Since the resolution of seven bridges of Königsberg problem (Euler 1741), the theory of networks, which deals with the study of complex interacting units represented as graphs, has demonstrated remarkable applications in various real-world systems (Albert and Barabási 2002). With an accelerated development in network science, various communities belonging to different branches of science, economics, biology, and sociology have witnessed growing applications of results and techniques of networks in their respective fields. The spectra of the adjacency matrix of a network have been shown to provide information about various structural properties of the network, as well as the dynamical behavior of the corresponding complex system. For example, the degeneracy of the *zero* and *one* eigenvalues provide a clue to the structural symmetries of the underlying networks (Yadav and Jalan 2015). The largest eigenvalue, in addition to capturing the information of the largest degree, is related to the synchronization phenomena of diffusively coupled dynamical units on the network (Restrepo et al. 2005). Further, spectra plays a pivotal role in determining the epidemic threshold of a disease outbreak (Van Mieghem et al. 2008), stability of a system (May 1972), drug identification in complex diseases (Rai et al. 2018), for studying international trade networks (Alhomaidhi et al. 2019) etc. Coupled dynamical evolution on networks can be better understood by the spectra of corresponding Laplacian matrices (Liu et al. 2015). Further, spectra of complex networks

have also been studied under the Random matrix theory framework (Jalan and Bandyopadhyay 2007; Erdős et al. 2012). Recently, in Susca et al. (2020), a technique has been proposed to compute the statistics of the second largest eigenvalue and the components of the corresponding eigenvector for sparse symmetric matrices. It is to be noted that various structural properties of networks are computationally hard to determine nevertheless, often, the spectral measures cater good insights into a network structure, and these spectral measures are computationally easier to calculate. For example, calculating various expansion properties of networks is computationally NP-hard in nature. However, fortunately, these properties are closely related to the second largest eigenvalue that we can calculate very fast (in $O(n^3)$, where n is the number of nodes in the network) (Alon 1995). Note that, though calculating spectra analytically is a troublesome task, there exist analytical approaches to calculate spectra for a few specific networks (Newman et al. 2019; Peixoto 2013; Newman 2019). Further, the expansion properties of graphs have found their applications in computational complexity theory (com 1980), for the determination of robustness of computer networks (Motwani and Raghavan 1995), graph pebbling, parallel sorting algorithms, and theory of error-correcting codes (Hoory et al. 2006), derandomization of random algorithms, analysis of algorithms in computational group theory, quantum cryptography, etc. Further, the second eigenvalue of the Laplacian matrix of a network is equivalent to its algebraic connectivity, also known as the Fiedler eigenvalue (Bapat 2010). Random regular networks form one very important class of networks and have been investigated intensively (Bender 1974; Bender and Canfield 1978; Bollobás 1980; McKay 1984; Wormald 1981), and for these networks, the second largest eigenvalue of the adjacency matrices is equivalent to the algebraic connectivity. If the second eigenvalues of these networks is lesser than their degrees, these networks are connected (Fiedler 1973). To get an overview of second largest eigenvalue, it is worth to see Dehmer and Emmert-Streib (2009), Van Mieghem (2010), Chung (1994).

Most of the studies on the second largest eigenvalue (λ_2) are done for random regular graphs, with sporadic studies for other networks. All these studies suggest that λ_2 can yield a good insight into properties of the underlying network structure (Marcus et al. 2013). Particularly, the suitability of a network for a specific application depends on λ_2, and often a small value of λ_2 is desirable (Hoory et al. 2006). Several classes of networks (graphs) are defined by the value the second largest eigenvalue take, for instance, reflexive graphs or hyperbolic graphs ($\lambda_2 \leq 2$), Salem graphs ($\lambda_2 \in [-2, 2]$), k-regular Ramanujan graphs ($\lambda_2 \leq 2\sqrt{d-1}$) (Hoory et al. 2006; Maxwell 1978). Further, the second eigenvalue is crucial in the dynamics of the Markov chain. It is found that networks with small λ_2 rapidly mix for reversible Markov chain yielding a high rate of information diffusion in large networks (Desai and Rao 1993).

The article is organized as follows. "Relationship of spectra with structure of networks" section presents results for various analytical relationships between the network's structural properties and their spectral measures. "Results on various network models" section focuses on the results on few popular model networks, namely, 1D lattice, Erdös-Renýi (ER) random, Scale-free networks and small-world networks. Exact analytical results are presented for 1D lattice model and $k-$random regular graphs, and numerical results are for other model networks. "Conclusion" section concludes the article.

Relationship of spectra with structure of networks

Let $G = (V, E)$ be a network on N nodes, where V, E are the vertex-set and edge-set, respectively. If two distinct vertices $i, j \in V$ are adjacent, we write $i \sim j$, otherwise, $i \not\sim j$. We represent network G by its adjacency matrix $A = (a_{ij})_{N\times N}$ defined as follows.

$$a_{ij} = \begin{cases} 1 & \text{if } i \sim j, \\ 0 & \text{otherwise.} \end{cases}$$

The eigenvalues of the adjacency matrix A are denoted by $\{\lambda_1, \lambda_2, \lambda_3, \ldots, \lambda_N\}$ where $\lambda_1 \geq \lambda_2 \geq ... \geq \lambda_N$. For un-directed and unweighted networks, A is a symmetric matrix with all eigenvalues being real. The set of the eigenvalues $\{\lambda_1, \lambda_2, \ldots, \lambda_N\}$ is known as the spectra of the network G. It is important to note that λ_1 for adjacency matrix having all non-negative entries is always positive, and for connected networks, $\lambda_1 > \lambda_2$ due to Perron-Frobenius Theorem. Let $\langle k \rangle$ denote the average degree of G, and $k_{\max}$ denote the maximum degree of G. The largest eigenvalue λ_1 satisfies $\langle k \rangle \leq \lambda_1 \leq k_{\max}$ (Sarkar and Jalan 2018). Also $\lambda_1 \leq \left(\frac{2M(N-1)}{N}\right)^{\frac{1}{2}}$, where M, N are the number of edges and nodes in the graph, respectively. If G is connected, then $\chi(G) \leq 1 + \lambda_1(G)$, where $\chi(G)$ is the chromatic number of G (Bapat 2010). The chromatic number $\chi(G)$ of graph G is the minimum number of colors required to color the vertices such that adjacent vertices get distinct colors. However, finding the chromatic number of a graph is an NP-hard problem.

Next, we see that along with λ_1, other eigenvalues of A implicate the following information about the structure of graph G (Bapat 2010).

1 $\lambda_1^2 + \lambda_2^2 + \cdots + \lambda_N^2 = 2M.$
2 $\sum_{i,j,i\neq j} \lambda_i \lambda_j = -M.$
3 $\lambda_1^3 + \lambda_2^3 + \cdots + \lambda_N^3 = 6|T|,$

where T is the set of all the cycles of length 3 in G (also referred as triangles). In general, the number of closed walks of length k in G equals $\sum_i^N \lambda_i^k$. A walk of length k in a graph G is a sequence of vertices $(v_1, v_2, \ldots, v_{k+1})$ such that there is an edge $v_i \sim v_{i+1}$ for $i = 1, 2, \ldots, k$. The walk is closed if $v_1 = v_{k+1}$.

In particular when G is random regular graph, λ_2 shares an interesting relationship with the expansion coefficient of G and its diameter. The expansion coefficient of G, denoted as $h(G)$ is defined as follows:

$$h(G) = \min_{0<|S|\leq N/2} \frac{E(S, \bar{S})}{|S|}, \tag{1}$$

where $S \subset V$, and $E(S, \bar{S})$ are the set of the edges with one end in S and other in $\bar{S}$. Alon and Milman (Hoory et al. 2006) proved that if G is a k-random regular graph,

$$\frac{k - \lambda_2}{2} \leq h(G) \leq \sqrt{2k(k - \lambda_2)}. \tag{2}$$

This immediately gives the following bounds on λ_2.

$$k - 2h(G) \leq \lambda_2 \leq k - \frac{h(G)^2}{2k}. \tag{3}$$

Nilli (Nilli 1991) proved that if a k-random regular graph has a diameter D, then

$$\lambda_2 \geq 2\sqrt{k-1}\left(1 - \frac{2}{D-2}\right) + \frac{2}{D-2} \tag{4}$$

Results on various network models

The relation (Eqs. 2–4) is valid for random regular networks, i.e., for networks with each node having the same degree. However, the second largest eigenvalue of the adjacency matrices of non-regular networks has not been given much attention. We numerically investigated the behavior of λ_2 for various model networks, namely, Erdös-Renýi (ER) random, scale-free, 1D lattice (for completeness), and small-world networks. ER random networks are constructed using the ER model ? as follows. Starting with N nodes, each pair of the nodes is connected with a probability $p = \langle k \rangle / N$. Our analysis has considered connected networks only without self-loops and multiple edges. The degree distribution of ER random networks follows a binomial distribution. Scale-free networks are constructed using BA preferential attachment method (Barabási and Albert 1999) in which each node prefers to connect with the existing higher degree nodes. Starting with a network with m_0 nodes, we start adding a new node at each time step having m connections such that $m \leq m_0$. The new nodes can be connected to any existing node, and to incorporate preferential attachment, the probability of it getting connected to the ith nodes is proportional to k_i where k_i is the degree of the ith node. Thus, after t time steps, the network will have $t + m_0$ nodes and mt edges. The network evolves into a scale-free network with degree distribution following a power law, that is, $P(k) \sim k^{-\gamma}$ where $\gamma = 3$. The 1D lattice considered here consists of a ring lattice with each node connecting exactly with the same number of neighbors on both sides. We construct small-world networks using the Watts and Strogatz algorithm (Watts and Strogatz 1998) as follows. Starting with a 1D lattice in which all the nodes have an equal degree, we rewire each edge of the network with a probability p_r. This procedure of the rewiring allows to transform a 1D lattice with $p_r = 0$, to a random network with $p_r = 1$. In the intermediate p_r values, the network manifests the small-world behavior, which is quantified by a very small average shortest path length.

First, we discuss available analytical results for λ_1 and λ_2, followed by numerical results for different model networks for various network parameters. The variation on λ_2 is compared with that of λ_1. As discussed earlier that λ_1 is bounded below by the average degree, and above by k_{max}, hence, an increase in the average degree will result in an increase in the lower bound of λ_1. In particular, for a k-random regular network λ_1 increases linearly with the average degree as $\langle k \rangle = k_{max} = \lambda_1$. However, λ_2 behaves quite differently. Figure 1 presents the behavior of λ_1 and λ_2 with respect to the average degree for various model networks. The value of λ_1 increases with the average degree for all the networks. In particular, for 1D lattice in (Fig. 1a) $\lambda_1 = \langle k \rangle$, it is easy to see that the all-one vector $\mathbf{1} = [1, 1, \ldots, 1]^T$ of order $N \times 1$ satisfy $A\mathbf{1} = \langle k \rangle \mathbf{1}$. Since A is an non-negative matrix and $\mathbf{1}$ is an non-negative vector, using Perron-Frobenius

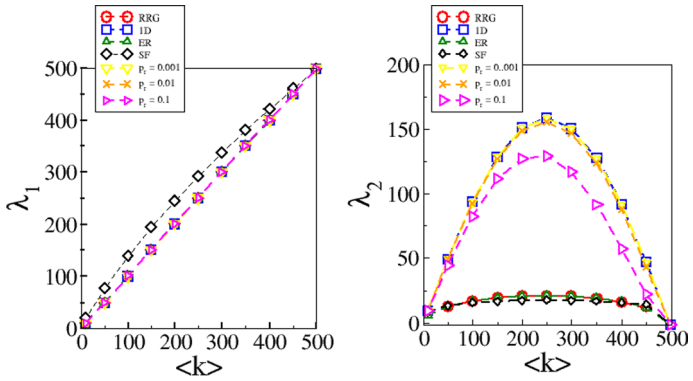

Fig. 1 Comparison of λ_1 and λ_2 for various model networks as a function of $\langle k \rangle$ with $N = 500$ for 20 different network realizations

theorem, λ_1 is the largest eigenvalue which is equal to $\langle k \rangle$. The second largest eigenvalue of a 1D lattice G on N nodes and having degree k is given by $\sum_{j=1}^{\frac{k}{2}} 2\cos\frac{2\pi j}{N}$. This can be seen as follows. Each node in G has an edge with each of immediate previous, next $\frac{k}{2}$ nodes. The first row of the adjacency matrix A of G is the following

$$0, \overbrace{1, \ldots, 1}^{\frac{k}{2}}, 0, \ldots, 0, \overbrace{1, \ldots, 1}^{\frac{k}{2}}.$$

The i-th row of A is the row-vector resulting after $i-1$ right shift of the first row. Thus A is a circulant matrix (for more detail on circulant matrices see (Gray 2006)). The eigenvalues of circulant matrix of order N with the first row as $c_0, c_1, \ldots, c_{n-1}$ are given by $\lambda_i = \sum_{j=0}^{N-1} c_k e^{\frac{-2\pi ij}{N}}$, for $i = 0, 1, \ldots, N-1$. The imaginary part cancels out because the adjacency matrix is symmetric, hence it will have only real eigenvalues. So we are left with only cos terms, which implies, $\lambda_i = \sum_{j=1}^{\frac{k}{2}} 2\cos\frac{2\pi ji}{N}$, for $i = 0, 1, \ldots, N-1$. Thus $\lambda_2 = \sum_{j=1}^{\frac{k}{2}} 2\cos\frac{2\pi j}{N}$, which follow the trend as is seen in Fig. 1b shown in blue.

For k-random regular networks, $\lambda_1 = k$. For ER random networks, $\lambda_1 \approx [1 + o(1)]\langle k \rangle$ (Chung et al. 2004). For scale-free networks, $\lambda_1 \approx \sqrt{k_{\max}}$ if $\gamma > 2.5$ and $\lambda_1 \approx \frac{\langle k^2 \rangle}{\langle k \rangle} = \frac{\sum_{i=1}^{N}(k_i)^2}{\sum_{i=1}^{N}(k_i)}$ if $2 < \gamma < 2.5$ (Sarkar and Jalan 2018). With increase in the average degree, λ_1 exhibits a consistent increase for all these networks. However, by keeping the network size fixed, as we increase the average degree of a network, λ_2 first exhibits an increase until $\langle k \rangle \sim N/2$, which is not surprising as λ_1 also exhibits an increase and one can expect of a similar trend followed by the second largest eigenvalue. However, rather intriguingly, if we increase the average degree further, λ_2 reflects a decreasing behaviour with $\langle k \rangle$. The trend of λ_2 is symmetric with respect to $\langle k \rangle = N/2$ (Fig. 1b).

We consider k-random regular networks for analytically substantiating this behaviour observed numerically for ER and SF networks. Let G be a k-random regular network on N nodes and M edges. Let $\{\lambda_1, \lambda_2, \lambda_3, \ldots, \lambda_N\}$ be the eigenvalues of the adjacency matrix of G such that $k = \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N$ hold. Since

$$\lambda_1^2 + \lambda_2^2 + \cdots + \lambda_N^2 = 2M.$$

Dividing both the sides by N we get

$$\frac{\lambda_1^2}{N} + \frac{\lambda_2^2}{N} + \cdots + \frac{\lambda_N^2}{N} = \frac{2M}{N} = \langle k \rangle = k. \tag{5}$$

We have

$$\frac{\lambda_2^2}{N} + \cdots + \frac{\lambda_N^2}{N} = \frac{2M}{N} = k - \frac{k^2}{N}. \tag{6}$$

Since N is constant, the quantity $k - \frac{k^2}{N}$ depends on the higher-order terms in L.H.S of the Eq. 6. The quantity $k - \frac{k^2}{N}$ first increases till k becomes $\frac{N}{2}$, followed by a decrease, and so does the higher-order terms. Therefore, λ_2 after reaching the threshold value starts decreasing.

For any other random network, the explanation is similar to what we deduced for random regular networks. Let G be any random network, for which Eq. 6 becomes

$$\frac{\lambda_2^2}{N} + \cdots + \frac{\lambda_N^2}{N} = \frac{2M}{N} = \langle k \rangle - \frac{\lambda_1^2}{N}. \tag{7}$$

Since $\langle k \rangle \leq \lambda_1 \leq \Delta$, where Δ is the largest degree in G. The RHS of Eq. 7 first takes increasing value till k becomes $\frac{N}{2}$, followed by a decrease, and so does λ_2 and the higher order terms.

Further, in Fig. 2, the plots are shown for $\frac{\lambda_2}{N}$ vs $\frac{\langle k \rangle}{N}$ for various network models. The behaviour is similar to what it is for λ_2 vs $\langle k \rangle$ as shown in Fig. 1. The ratio $\frac{\lambda_2}{N}$ increases when $\frac{\langle k \rangle}{N}$ increases from 0 to 0.5 and after that it shows a decreasing trend from 0.5 to 1. In every iteration, for 1D lattice, we have plot for double the size of previous network instance, but keeping $\frac{\langle k \rangle}{N}$ fixed. We see that these curves overlaps which can be explained as follows. The second largest eigenvalue of 1D lattice with degree k is $\lambda_2 = \sum_{j=1}^{\frac{k}{2}} 2\cos\frac{2\pi j}{N}$. For a given N and k, expanding the summation, we get the following expression

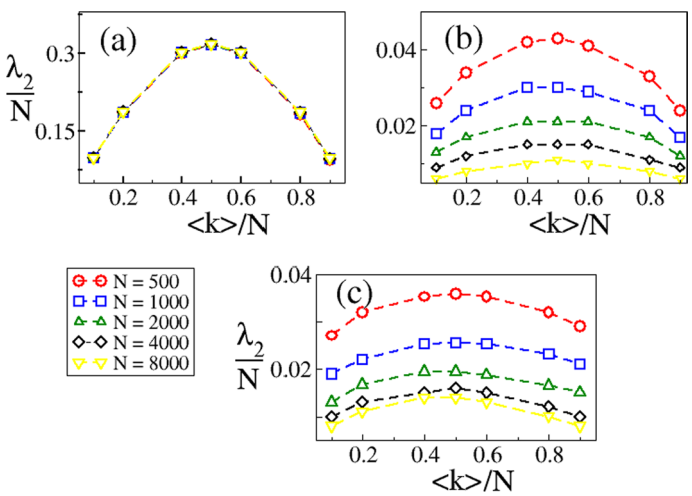

Fig. 2 Plot of λ_2/N as a function of $\langle k \rangle/N$ for various model networks. **a** 1D, **b** ER, **c** SF

$$\lambda_2 = 2\Big(\cos\frac{2\pi}{N} + \cos\frac{4\pi}{N} + \cos\frac{6\pi}{N} + \cdots + \cos\frac{\pi k}{N}\Big) \tag{8}$$

Now let us change the parameters N, k to N', k', respectively such that $\frac{k}{N} = \frac{k'}{N'}$. Let the corresponding second largest eigenvalue for these parameters be λ_2'. We can express λ_2' in terms of N and k as follows. We have $N' = 2N$ and so $k' = 2k$, then

$$\lambda_2' = 2\Big(\Big(\cos\frac{2\pi}{N} + \cos\frac{\pi}{N}\Big) + \Big(\cos\frac{4\pi}{N} + \cos\frac{3\pi}{N}\Big) + \cdots + \Big(\cos\frac{\pi k}{N} + \cos\frac{\pi(k-1)}{N}\Big)\Big) \tag{9}$$

Next, we have to prove that $\frac{\lambda_2'}{N'} = \frac{\lambda_2}{N}$, that is, R.H.S of Eq. 9 should be equal to 2 times R.H.S of Eq. 8 as $N' = 2N$. The consecutive terms of Eq. 9 (enclosed in parentheses) can be written as $\cos\frac{\pi j}{N} + \cos\frac{\pi(j-1)}{N}$ where $j = 2, 4, 6, \ldots, k$. The second term can be further written as $\cos(\frac{\pi j}{N} - \frac{\pi}{N})$. Since $\cos\theta$ is a continuous function and $\cos(\theta - \delta) \approx \cos\theta$ when $\delta \to 0$, we have $\cos(\frac{\pi j}{N} - \frac{\pi}{N}) \approx \cos(\frac{\pi j}{N})$ for $N \to \infty$. Thus, R.H.S of Eq. 9 becomes $4 \times (\cos\frac{2\pi}{N} + \cos\frac{4\pi}{N} + \cos\frac{6\pi}{N} + \cdots + \cos\frac{\pi k}{N})$, which proves that $\frac{\lambda_2'}{N'} = \frac{\lambda_2}{N}$.

Expansion coefficient $h(G)$ of random regular graphs and λ_2

The expansion coefficient $h(G)$ of a network G reveals how well the network is connected. For a disconnected network $h(G) = 0$, and higher the expansion coefficient better well-connected a network is. This can be directly spotted from the expression for the expansion coefficient

$$h(G) = \min_{0<|S|\le N/2} \frac{E(S,\bar{S})}{|S|}. \tag{10}$$

This means that for any subset S, the number of edges from S to the rest of the vertices is at least $h(G) \times \min(|S|, |\bar{S}|)$. Therefore, the higher the value of $h(G)$ more well-connected the network is. However, in general calculating $h(G)$ is an intractable problem (NP-hard) (Hoory et al. 2006). Nevertheless, for a 1D lattice, we can easily calculate the expansion coefficient as follows. Consider a 1D lattice of degree k on N nodes. By Eq. 10, the minimum ratio is achieved for $|S| = \frac{N}{2}$. It is easy to observe that the total number of edges from S to rest of the vertices are

$$E(S,\bar{S}) = 2 \times \Big(1 + 2 + \cdots + \frac{k}{2}\Big).$$

Hence,

$$h(G) = \frac{k}{N} \times \Big(\frac{k+2}{2}\Big).$$

Figure 3 plots λ_2 of 1D lattice against the lower and upper bounds in terms of $h(G)$ (Expression 3). It can be seen that the lower bound almost matches the behaviour of λ_2 given by the Inequality 2

$$\frac{k-\lambda_2}{2} \le h(G) \le \sqrt{2k(k-\lambda_2)}.$$

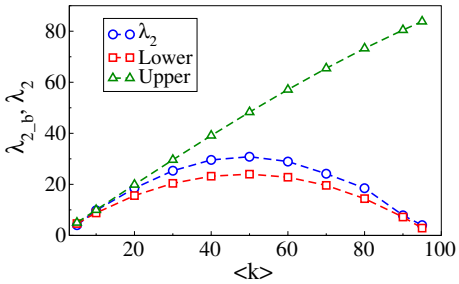

Fig. 3 Numerical value of λ_2 (blue) for 1D lattice with $k/2$ nearest neighbour couplings, its upper (green) and lower bound (red) as a function of the average degree. Here, $N = 100$

by Definition 1, in general for any k-random regular network G, the expansion coefficient $h(G)$ will increase as k increases, thus the quantity, $k - \lambda_2$ (it is present in both the sides of inequality, also known as spectral gap) must also increase with k. However, in general, calculation of $h(G)$ is NP-hard, it will be interesting to check how λ_2 behaves with respect to $h(G)$ for other networks (Hoory et al. 2006).

Conclusion

This article reviews the properties of the second largest eigenvalue for 1D lattice, random regular graphs and networks capturing properties of real-world complex systems. The intriguing conclusion of future interests is that λ_2 behaves in a completely different demeanor from the largest eigenvalues. The largest eigenvalue λ_1 is more dependent on the highest degree of the corresponding networks. The larger the value of k_{max}, the higher will be the value of λ_1, however λ_2 though having an upper bound of k_{max} turns out to be independent of it. For model networks, an increase in the average degree leads to an increase in the value of λ_1. However, contrarily λ_2 first manifests an increase till $\langle k \rangle = \frac{N}{2}$ followed by a decreasing trend. Further, λ_1 of the scale-free networks is always higher than the 1D lattice and random network since it has higher k_{max} while λ_2 is higher for 1D lattice than that of the random and scale-free networks. We have analytically obtained the lower bound of λ_2 for 1D lattice using its relation with the expansion coefficient and found that the numerical value of λ_2 follows the same behavior as its lower bound.

Abbreviations

ER	Erdös–Renýi
SF	Scale-free
RRG	Random regular graph
BA	Barabási and Albert
L.H.S	Left hand side
R.H.S	Right hand side

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Author contributions
AM, RS and SJ designed the study and the methodologies, AM and RS processed and analysed the results. All the Authors wrote and approved the manuscript.

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