Ensemble averageability in network spectra

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The extreme eigenvalues of connectivity matrices govern the influence of the network structure on a number of network dynamical processes. A fundamental open question is whether the eigenvalues of large networks are well represented by ensemble averages. Here we investigate this question explicitly and validate the concept of ensemble averageability in random scale-free networks by showing that the ensemble distributions of extreme eigenvalues converge to peaked distributions as the system size increases. We discuss the significance of this result using synchronization and epidemic spreading as example processes.

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The structure and dynamics of complex networks is of increasing interest in nonlinear dynamics, biological physics, complex systems, and statistical physics. Part of this interest comes from the realization that commonly observed structural properties, such as the scale-free (SF) degree distribution, strongly influence the collective dynamics of the system. In many dynamical processes, the influence of the network structure is encoded in the extreme eigenvalues of a connectivity matrix. In complete synchronization and consensus phenomena, for example, the stability and convergence are often determined by the largest and smallest nonzero eigenvalues of the Laplacian matrix. In diffusion processes, the relaxation rate is governed by the corresponding eigenvalues of the normalized Laplacian. The largest eigenvalue of the adjacency matrix, on the other hand, plays a central role in determining epidemic thresholds and critical couplings for the onset of coherent behavior.

Our ultimate goal is to find a way to determine the extreme eigenvalues (and thereby the dynamics) of networks by only using averages and local information about the network structure. This problem is properly defined for ensembles of networks and involves two elements: determination of the ensemble averages and characterization of the fluctuations across the ensemble. Previous studies on ensemble averages have focused on spectral densities and applications, while here we focus on the extreme eigenvalues. In this case, the study of fluctuations is crucial to assess how well the averages reflect the properties of individual networks in the ensemble. The broader the distributions of extreme eigenvalues across the ensemble, the more limited the information provided by the averages will be. It has been suggested recently that the degree distribution and other statistical properties are not sufficient to characterize the eigenvalues of random SF networks.

Though the spectral properties of these networks are different from those traditionally considered in random matrix theory, as far as we know, extreme eigenvalue distributions have not been studied for network ensembles and their statistical properties remain essentially unknown.

In this Letter, we investigate the averageability of the extreme eigenvalues in ensembles of random SF networks. We define a quantity to be ensemble averageable if the variance of its probability distribution goes to zero in the limit of large system size. We show that the largest eigenvalues of the Laplacian and adjacency matrices are determined mainly by the largest degree node of the network, while the smallest nonzero eigenvalue of the Laplacian depends on the details of the way in which nodes are connected. We provide strong evidence that the smallest nonzero eigenvalue of the Laplacian and both extreme eigenvalues of the normalized Laplacian are ensemble averageable. That is, as the number of nodes increases, the distributions become increasingly more peaked and the averages provide increasingly more accurate information about the behavior of most networks in the ensemble. We apply these findings to the study of synchronization and epidemic spreading. We show that the physical quantities characterizing the dynamics are averageable and properly represented by functions of the averages of the extreme eigenvalues. This provides an unambiguous spectral characterization of the dynamics in ensembles of large-size networks.

We focus on undirected random SF networks with the constraints of having a single connected component and no self- or multiple links. Starting with a graph degree sequence for $N$ nodes generated from a power-law distribution $P_d(k) = c_d k^{-\gamma}$ with $k \geq k_0$, where $c_d \approx (\gamma - 1) k_0^{\gamma-1}$ for large $N$, we construct an initial network satisfying the given constraints. Then, we randomize the network topology using the degree-preserving algorithm of Ref. to implement $(\sum_i k_i)^2$ link-rewirings, while keeping the constraints by rejecting constraint-breaking rewirings. The only degree correlations in the network construction are those due to these constraints (see, for example, Ref. ). We focus on the ensemble of all such networks. We consider three connectivity matrices of broad interest: the adjacency matrix $A$, defined as $A_{ij} = 1$ if nodes $i$ and...
j \neq i are connected and \( A_{ij} = 0 \) otherwise; the Laplacian \( L \equiv D - A \) and the normalized Laplacian \( \bar{L} \equiv D^{-1}L \), where \( D = \text{diag}\{k_1, \ldots, k_N\} \) is the diagonal matrix of degrees. For undirected networks, all the eigenvalues of these matrices are real. The eigenvalues of \( L \) and \( \bar{L} \) can be ordered as \( \lambda_1 = 0 = \lambda_2 \leq \cdots \leq \lambda_N \) and \( \mu_1 = 0 < \mu_2 \leq \cdots \leq \mu_N \leq 2 \), respectively. The largest eigenvalue of \( A \) is positive and is denoted by \( \lambda_N \). The nodes are labeled in increasing order of their degrees \( k_i \), such that \( k_1 \leq k_2 \cdots \leq k_N \).

For the Laplacian \( L \), we estimate the largest eigenvalue \( \lambda_N \) by using nondegenerate perturbation theory \([21]\). In \( L = D - A \), we consider \( D \) as an unperturbed matrix and \( -A \) as a perturbation. This decomposition leads to the perturbation expansion of \( \lambda_N \), which up to second order of \( A \) is:

\[
\lambda_N \approx k_N - A_{NN} + \sum_{j \neq N} \frac{(A_{Nj})^2}{k_N - k_j} \approx k_N + 1. \tag{1}
\]

Here we have used the fact that the second order term can be expanded as \( \sum_j (A_{Nj})^2 \frac{k_j}{k_N - k_j} = 1 + \frac{1}{k_N} + \cdots \), where \( k_N^{(1)} \) is the average degree of the nearest neighbors of node \( N \). In uncorrelated SF networks, \( k_N^{(2)}/k_N \approx k_N^{-1} \sum_i k_i^2 P_i(k) \ll 1 \) for \( \gamma > 2 \) and large \( N \) \([22]\), which leads to \( \lambda_N \approx k_N + 1 \) for large \( N \). This result is quite neat since \( \lambda_N \) of any network is lower bounded by \( k_N + 1 \) \([22]\). The same approach can also be used to predict a power-law tail for the \( \lambda \)-density, \( \rho(\lambda) \sim \lambda^{-\gamma} \) \([24]\), because \( \lambda_1 \approx k_1 \) is still valid for other nondegenerate \( k_i \)'s in the tail of \( P_d \sim k^{-\gamma} \). Similarly, we can also obtain the largest eigenvalue \( \Lambda_N \) of the adjacency matrix by considering the largest diagonal term of matrix \( A^2 \), given by \( k_N \), and regarding the off-diagonal elements as a perturbation. Under the approximation of local tree-like structure, we obtain \( \Lambda_N^2 \approx k_N + k_N^{(1)} - 1 \), which provides a second-order correction to the previous result \( \Lambda_N^2 \sim k_N \) \([12, 13, 14]\).

Equation (1) implies that \( \lambda_N \) depends on the specific realization of the degree sequence, which fluctuates widely across the ensemble. For \( N \) integers randomly generated from \( P_d(k) \), the asymptotic form of the probability distribution of the largest one, \( k_N \), is given by the Fréchet distribution \( P(k_N) \sim c_0 N k_N^2 \exp[-N(k_N^{(1)}/k_N)^{\gamma-1}] \) \([23]\). The average of \( k_N \) can be obtained from \( P(k_N) \) as \( \langle k_N \rangle \approx k_0 N^{\gamma-1} \exp\left[\frac{\gamma - 1}{\gamma} \left(\frac{k_0}{k_N} - 1\right)^{\gamma-1}\right] \), where \( \Gamma(a, b) \) denotes the Incomplete Gamma Function. The standard deviation of \( P(k_N) \) increases as \( \sim N^{\gamma-2} \) in the same way as \( \langle k_N \rangle \) does. This implies that \( k_N \), and hence \( \lambda_N \), are not averageable quantities in this ensemble.

Instead, the corresponding ensemble averageable quantity is the reduced largest eigenvalue \( \tilde{\lambda}_N \equiv \lambda_N/(k_N + 1) \). While \( \lambda_N \) may deviate from the prediction in Eq. (1), the numerical calculation confirms that, as \( N \) grows, the distribution of \( \tilde{\lambda}_N \) becomes extremely peaked, as shown in Fig. 1. This indicates that \( \lambda_N \) of large random SF networks is accurately determined exclusively by \( k_N \), which involves local information only.

On the other hand, we find that \( \lambda_2, \mu_2 \) and \( \mu_N \) are ensemble averageable by themselves. As shown in Fig. 2, these eigenvalues have bell-shaped distributions with well-defined averages in the ensemble of SF networks. We note that the statistics of \( \mu_N \) is indistinguishable from that of \( 2 - \mu_2 \). More important, we find that \( P(\lambda_2) \) and \( P(\mu_2) \) converge to increasingly peaked distributions as \( N \) increases. We have confirmed this behavior by analyzing the \( N \)-dependence of the standard deviation, which decreases with increasing \( N \). This indicates that the probability of having large deviations from the averages decreases to very small values as the size of the system increases. Therefore, for large \( N \), the eigenvalues \( \lambda_2, \mu_2 \) and \( \mu_N \) of most networks in the ensemble are well represented by the ensemble averages.

To provide approximate bounds for the ensemble averages, we derive an approximation for the extremes of the spectral density of uncorrelated tree-like networks in the thermodynamic limit. For the Laplacian \( L \), the spectral density is given by \( \rho(\lambda) = -\frac{1}{N} \text{Im} \left( \frac{1}{\text{Tr} \left( e^{-L} \right)} \right) \) and can be analyzed using a weighted version of the random walk method \([13, 26]\) with a multiplying weight factor of \( [k_j - (\lambda + i0^+)]^{-1} \). This leads to \( \rho(\lambda) \sim \frac{1}{N} \text{Im} \left( \frac{1}{\text{Tr} \left( e^{-L} \right)} \right) \).
\[ \frac{1}{\pi} \text{Im} \sum_k \frac{P_d(k)}{k - \lambda - i\omega + i\eta T(k)} \text{, where } T(\lambda) \text{ satisfies } T(\lambda) = \frac{1}{i(k)} \sum_k \frac{kP_d(k)}{k - \lambda - i\omega + i\eta T(k)} \text{, with } \langle k \rangle = \sum_k kP_d(k). \]

To obtain the lower extreme \( \lambda^- \) we note that \( T \) is complex (so that \( \rho(\lambda) > 0 \)) if \( \lambda > \lambda^- \), and \( T \) is real (so that \( \rho(\lambda) = 0 \)) if \( \lambda < \lambda^- \). Then, for real \( x \equiv \sqrt{\frac{k}{\pi}} \) such that \( g(x) \equiv \frac{1}{(k)} \sum_k \frac{kP_d(k)}{k + x} \leq 1 \), we obtain

\[
\lambda^- \simeq \max_x \left[ \frac{1}{2} \left( x + 1 + |x - 1| \sqrt{1 - g(x)} \right) \right]. \tag{2}
\]

For the normalized Laplacian \( L \), it is known [13] that the spectral density is given by \( \rho(\nu) \simeq -\frac{1}{\pi} \text{Im} \sum_k \nu \frac{P_d(k)}{k - \lambda + i\eta T(\nu)} \text{, with } T(\nu) \text{ satisfying } T(\nu) = \frac{1}{i(k)} \sum_k \frac{kP_d(k)}{k - \lambda + i\eta T(\nu)} \text{, where } \nu \equiv 1 - \mu. \) From the identity \( T^*(\nu) = -T(-\nu) \) we obtain the spectral symmetry \( \rho(\nu) \simeq \rho(-\nu) \), which helps explain our numerical result \( \langle \mu_N \rangle \simeq 2 - \langle \mu_2 \rangle \) (cf. Fig. 2). We then obtain an approximate expression for the upper (lower) extreme \( \mu^+ \) (\( \mu^- \)) by using the same argument used to derive Eq. 2. For real \( x \equiv T/\nu \),

\[
[1 - \mu^\pm]^2 \simeq \min_{0 < x < 1} \left[ \frac{1}{(k)x} \sum_k kP_d(k) \right] \bigg/ \sum_k k - (k - 1)x \right]. \tag{3}
\]

If \( k_0 \) is large, the r.h.s. of Eq. (3) approaches \( \sum_k 4(k - 1)P_d(k)/(k(k)) \) and \( \mu^\pm \simeq 1 \pm 2/\sqrt{k} \), which agrees with previous results for densely connected networks [14 24].

For the large but finite-size sparse networks of our interest, the actual ensemble average \( \langle \mu_2 \rangle \) is expected to fall inside of the pseudogap region \((0, \mu^-)\) because of the existence of extended tails of \( \rho(\mu) \) (see Ref. 27 for the case of homogeneous networks). Then, given a degree distribution, \( \mu^- \) serves as an approximate upper bound for \( \langle \mu_2 \rangle \). On the other hand, because all the networks in the ensemble have all degrees \( \geq k_0 \), the average \( \langle \mu_2 \rangle \) is expected to be lower bounded by the corresponding average of the ensemble of \( k \)-regular random graphs with degree \( k = k_0 \) for all the nodes, which is nonzero for \( k_0 \geq 3 \) 28. Thus, we can write \( \mu^- \lesssim \langle \mu_2 \rangle \lesssim \mu^- \) and, symmetrically, we have \( \mu^+ \lesssim \langle \mu_N \rangle \lesssim \mu^+ \), where \( \mu^\pm \) denotes \( \mu^\pm \) at \( \gamma = \infty \), representing \( k \)-regular graphs with \( P(k) = \delta(k - k_0) \). For \( \lambda_2 \), similar arguments lead to \( \lambda_2^- \lesssim \langle \mu_2 \rangle \lesssim \lambda^- \), where \( \lambda_2^- \) is \( \lambda^- \) at \( \gamma = \infty \). As shown in Fig. [3] the numerical results are in good agreement with these predictions.

We now use synchronization and epidemic spreading as example processes to show how our findings can impact the study of network dynamics. In the complete synchronization of identical oscillators, the ability of an oscillator network to synchronize is measured by the range of the coupling parameter for which synchronization is stable and is determined by \( R_\lambda \equiv \lambda_2 \) 3. If the input signal is normalized to be equal for all the oscillators, then the same stability condition is determined by \( R_\mu \equiv \mu_2 \) [8]. In epidemic spreading, on the other hand, the epidemic threshold of the susceptible-infected-susceptible model is determined by \( 1/\Lambda_N \) [4]. These dynamical processes, as well as many others, are determined by functions of the extreme eigenvalues. To characterize a process in SF networks, in principle one would have to average the corresponding function over all possible realizations of the networks or study the process on a case-by-case basis. We have shown, however, that the extreme eigenvalues are well represented by averages combined with local information. A practical question then is whether one can approximate the averages of the functions by functions of the average eigenvalues.

The average of a function, \( \langle f(x) \rangle \), is not necessarily equal to the function of the average, \( f(\langle x \rangle) \). However, from the identity 
\[
\sum_j f(x_j)/n = f(\sum_j x_j/n) \text{ for}
\]

\[ P(1/\Lambda) \text{, which agrees with } \hat{\Lambda}_N \text{ at } \gamma = \frac{4P(R_N)}{\sqrt{\Lambda}}. \]
$x_1 = x_2 = \cdots = x_n$, one expects that, if the distribution of $x$ goes to a $\delta$-like function in the thermodynamic limit, then $\langle f(x) \rangle$ approaches $f(\langle x \rangle)$. For finite $N$, this can be formalized for locally monotonic functions by noting that the probability distributions of the function and variable are related through $P_f(f(x)) = P_x(x)/df(x)dx$. If $f(x)$ can be expressed as a uniformly convergent Taylor series around $x = \langle x \rangle$, the deviation of $f(\langle x \rangle)$ from $\langle f(x) \rangle$ can be written as $\langle f(x) \rangle - f(\langle x \rangle) = \sum_{n=2}^{\infty} \frac{1}{n!} f^{(n)}(\langle x \rangle) \left( x - \langle x \rangle \right)^n$, where $f^{(n)}(\langle x \rangle)$ denotes the $n$th derivative of $f(x)$ at $x = \langle x \rangle$. In this case, the central moments $\langle (x - \langle x \rangle)^n \rangle$ determine the $N$-dependence of the deviation. If $x$ is averageable, this deviation is expected to decrease as $N$ increases and the central moments decrease.

In Fig. 4 we show numerically that the averages of the functions $R_{\lambda} \equiv R_{\lambda}/(k_N + 1)$, $R_{\mu}$, and $1/\Lambda_N$ are indeed well approximated by the functions of the average eigenvalues:

$$\langle R_{\lambda} \rangle \simeq \frac{\langle \lambda_N \rangle}{\langle \lambda_2 \rangle}, \quad \langle R_{\mu} \rangle \simeq \frac{\langle \mu_N \rangle}{\langle \mu_2 \rangle}, \quad \frac{1}{\Lambda_N} \simeq \frac{1}{\langle \Lambda_N \rangle}. \quad (4)$$

In the lower panels of Fig. 4 we show that the probability distributions of these functions become increasingly more peaked as $N$ increases, which indicates that the functions themselves are ensemble averageable. Note that we have normalized $R_{\lambda}$ to benefit from the fact that $\lambda_{\lambda}$ is averageable. The function $R_{\lambda}$ is broadly distributed in the ensemble but can be estimated for individual realizations of the network using $R_{\lambda} \approx (k_N + 1)/\langle R_{\lambda} \rangle$. A similar argument could be used for $1/\Lambda_N$, although in this case the extreme statistics of $x = k_N^{1/\alpha} \sim 1/\Lambda_N$ is directly given by the Weibull distribution $P(x) \propto x^{\gamma-3} \exp(-cn x^{2\gamma-2})$, which becomes increasingly peaked as $N$ increases.

The importance of our results is twofold. First, despite the rich variety of possible structural configurations of individual networks, one can conclude that most networks in an ensemble of large SF networks have remarkably similar spectral properties. Second, many network dynamical processes can be described using average eigenvalues and local information provided by the degrees, which require very few network parameters. These results have broad significance in view of the previous finding [10] that there are networks in the SF ensemble with very different extreme eigenvalues, implying large deviations in the corresponding dynamics. Our results show that the probabilities of such large deviations are remarkably small and decrease with the increasing size of the networks.

The averageability of the extreme eigenvalues established in this Letter helps provide an unambiguous setting for the spectral characterization of dynamical processes on ensembles of complex networks. For large random SF networks, our results show that the eigenvalues $\lambda_2$, $\mu_2$, and $\mu_N$ are statistically well characterized by the ensemble averages determined by the degree distribution, which is in sharp contrast with the conclusions drawn from the study of particular networks [10]. Our conclusion also applies to $\lambda_N$ and $\Lambda_N$ normalized by simple functions of the maximum degree. These results provide evidence of self-averaging properties reminiscent of the laws of large numbers and are likely to remain valid for other ensembles of disordered networks.

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