

Fundamental Structural Constraint of Random Scale-Free Networks

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We study the structural constraint of random scale-free networks that determines possible combinations of the degree exponent γ and the upper cutoff k_c in the thermodynamic limit. We employ the framework of graphicality transitions proposed by Del Genio and co-workers [Phys. Rev. Lett. **107**, 178701 (2011)], while making it more rigorous and applicable to general values of k_c . Using the graphicality criterion, we show that the upper cutoff must be lower than $k_c \sim N^{1/\gamma}$ for $\gamma < 2$, whereas any upper cutoff is allowed for $\gamma > 2$. This result is also numerically verified by both the random and deterministic sampling of degree sequences.

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Complex networks [1] are found in diverse natural and artificial systems, which consist of heterogeneous elements (nodes) coupled by connections (links) markedly different from those of ordinary lattices. In particular, many systems [2–6] can be interpreted as scale-free networks, in which the fraction of nodes with degree k (i.e., k links) obeys the power-law distribution $P(k) \sim k^{-\gamma}$ over a broad range of values bounded by $k_m \leq k \leq k_c$ where γ is called the degree exponent, k_m is the lower cutoff, and k_c is the upper cutoff. There have been interests in topological and dynamical properties induced by the degree distribution, which have been examined through various studies on random scale-free networks [7–13].

Random scale-free networks refer to an ensemble of networks constrained only by the parameters γ , k_m , and k_c . In general, k_m is set as a constant, while k_c is assumed to increase with the number of nodes N as $k_c \sim N^\alpha$ with $0 \leq \alpha \leq 1$. Besides, self-loops or multiple links between a pair of nodes are often disallowed. Under the circumstances, the degree exponent γ and the cutoff exponent α determine various properties of networks in the thermodynamic limit, $N \rightarrow \infty$. It is known that γ contributes to the resilience against node failures [7], the epidemic threshold [8], the consensus time of opinion dynamics [9], etc. Meanwhile, α affects the expected value of the generated maximum degree [10], degree correlations [11], finite-size scaling at criticality [12,13], etc.

The studies of random scale-free networks characterized by γ and α must be based on the knowledge that such networks actually exist in the thermodynamic limit. Hence, it is necessary to understand the constraint on the possible values of γ and α . This problem is exactly equivalent to the issue of the graphicality of random scale-free networks. A degree sequence $\{k_1, k_2, \dots, k_N\}$ is said to be *graphical* if it can be realized as a network without self-loops or multiple

links. As an indicator of the existence of graphical sequences, the graphicality fraction g [14] is defined as the fraction of graphical sequences among the sequences with an even degree sum generated by $P(k)$. Note that the degree sequences with an odd degree sum are left out, since such sequences are trivially nongraphical. The constraint on the possible values of γ and α can be obtained from the behavior of g due to the fact that the random scale-free networks with given γ and α exist in the thermodynamic limit if and only if g is nonzero as $N \rightarrow \infty$.

Using the graphicality criterion given by the Erdős-Gallai (EG) theorem [15], Del Genio and co-workers [14] have recently studied the behavior of g as a function of γ only for the special case of $k_c = N - 1$ and $k_m = 1$. They found

$$g = \begin{cases} 0 & \text{if } 0 \leq \gamma \leq 2 \\ 1 & \text{otherwise,} \end{cases}$$

where the abrupt changes of g at $\gamma = 0$ and $\gamma = 2$ were termed graphicality transitions [14]. This result implies that there exist only sparse random scale-free networks with a finite average degree ($\gamma > 2$) and left-skewed networks with an abundance of hubs ($\gamma < 0$) in the thermodynamic limit when the range of degree is kept maximal.

In this Letter, we generalize their study to arbitrary choices of degree cutoffs, so that we can provide the complete picture of the constraint on the possible values of γ and α . Starting from the EG theorem, we present a rigorous derivation of g as a function of both γ and α , which is then verified and supplemented by numerical results.

The EG theorem [15] states that a degree sequence sorted in the decreasing order $k_1 \geq k_2 \geq \dots \geq k_N$ is graphical if it has an even sum and satisfies the EG inequalities given by

TABLE I. Scalings with N of the n th largest degree k_n for arbitrary values of α , β , and γ .

	$\beta = 0$	$0 < \beta < 1$	$\beta = 1$
$\gamma < 1$	N^α	N^α	N^α
$\gamma = 1$	N^α	N^α	$k_n^\nu N^{\alpha(1-\nu)}$
$\gamma > 1$	$N^{\min[\alpha, 1/\gamma-1]}$	$N^{\min[\alpha, 1-\beta/\gamma-1]}$	N^0

$$\sum_{i=1}^n k_i \leq n(n-1) + \sum_{i=n+1}^N \min[n, k_i] \quad (1)$$

for any integer n in the range $1 \leq n \leq N-1$.

To determine whether those inequalities are satisfied in the thermodynamic limit, we derive the network-size scalings of the left-hand side (lhs) and the right-hand side (rhs) of each inequality. As the first step, we calculate the scaling of k_n from the cumulative mass function of k_n , which is denoted by $\Gamma_N^{(n)}$. The maximum degree ($n=1$) satisfies

$$\Gamma_N^{(1)}(k) = \prod_{i=1}^N \text{Prob}[k_i \leq k] = [C(k)]^N, \quad (2)$$

where C is the cumulative mass function of degree. Since $\Gamma_N^{(n)}$ satisfies the recursive relation

$$\begin{aligned} \Gamma_N^{(n)}(k) - \Gamma_N^{(n-1)}(k) &= \text{Prob}[k_{n-1} > k \text{ and } k_n \leq k] \\ &= \binom{N}{n-1} [1 - C(k)]^{n-1} [C(k)]^{N-n+1}, \end{aligned} \quad (3)$$

we can obtain its exact form as

$$\Gamma_N^{(n)}(k) = \sum_{i=0}^{n-1} \binom{N}{i} [1 - C(k)]^i [C(k)]^{N-i}. \quad (4)$$

Suppose $n = \nu N^\beta$, where $\nu > 0$ and $0 \leq \beta \leq 1$. If $\beta > 0$, we can use the following approximation for large N :

$$\Gamma_N^{(n)}(k) \approx \frac{\text{erf}\left\{\frac{N[C(k) + \nu N^{\beta-1} - 1]}{\sqrt{2NC(k)[1-C(k)]}}\right\} + 1}{2}. \quad (5)$$

Using Eq. (4) for $\beta = 0$ and Eq. (5) for $\beta > 0$, we can find the range of k in which $\Gamma_N^{(n)}(k)$ increases from 0 to 1 in the limit $N \rightarrow \infty$. Since the typical values of k_n must fall within this range of k , we can obtain the network-size scalings of k_n as listed in Table I.

While both sides of the EG inequalities are sums over k_n , we can approximate those sums as integrals, since it does not affect the the leading N -dependent term that determines the scaling relation. It is straightforward to approximate the lhs, while the rhs needs a careful reformulation. The second term of the rhs satisfies

$$\begin{aligned} \sum_{i=n+1}^N \min[n, k_i] &= N\theta(n - k_m) \sum_{k=k_m}^{\min[n, k_{n+1}]} kP(k) \\ &\quad + N\theta(k_{n+1} - n - 1) \sum_{\max[n+1, k_m]}^{k_{n+1}} nP(k), \end{aligned} \quad (6)$$

where θ denotes the Heaviside step function defined by $\theta(x) = 1$ if $x \geq 0$, and $\theta(x) = 0$ otherwise. From now on, each summation can be converted to an integral over the same range. Calculating all the integrals, we can single out the leading N -dependent terms of each side, as listed in Table II. The scalings of those terms are completely determined by the three exponents α , β , and γ , while the lower cutoff k_m turns out to be irrelevant.

We can now determine whether the EG inequalities are satisfied through the comparison of scaling exponents in both sides. By the EG theorem, $g = 1$ if the inequalities are satisfied for all possible values of β , and $g = 0$ if there exist the values of β at which some inequalities are violated. Hence, the asymptotic behavior of g is obtained as follows:

TABLE II. Scalings with N of each side of the n th EG inequality for arbitrary values of α , β , and γ .

	$\beta = 0$	$0 < \beta < 1$	$\beta = 1$
lhs	$\gamma < 1$	N^α	$N^{\alpha+\beta}$
	$\gamma = 1$	N^α	$N^{\alpha+\beta}$
	$1 < \gamma < 2$	N^α	$N^{\min[\alpha+\beta, 1+\alpha(2-\gamma)]}$
	$\gamma = 2$	N^α	$\min[N^{\alpha+\beta}, N \ln N]$
	$\gamma > 2$	$N^{\min[\alpha, 1/\gamma-1]}$	$N^{\min[\alpha+\beta, 1-(\gamma-2/\gamma-1)(1-\beta)]}$
rhs	$\gamma < 1$	N	$\max\{N^{2\beta}, N^{1+\min[\alpha, \beta]}\}$
	$\gamma = 1$	N	$\max\{N^{2\beta}, \min[\frac{N^{1+\alpha}}{\ln N}, N^{1+\beta}]\}$
	$1 < \gamma < 2$	N	$\max\{N^{2\beta}, N^{1+\min[\alpha, \beta](2-\gamma)}\}$
	$\gamma = 2$	N	$\max[N \ln N, N^{2\beta}]$
	$\gamma > 2$	N	$\max[N, N^{2\beta}]$

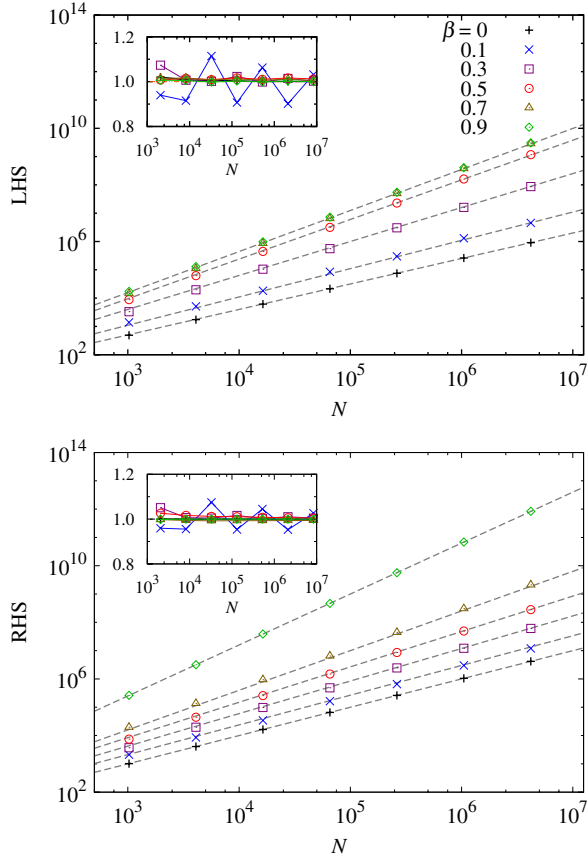


FIG. 1 (color online). N dependence of the n th EG inequality obtained from 10^3 random degree sequences (symbols) for $\gamma = 1.5$ and $\alpha = 0.9$. It is in good agreement with the scalings (lines) predicted in Table II, which is also confirmed by the insets. The ratio between the successive slopes of each symbol and the slope of the corresponding line stays close to one.

$$g = \begin{cases} 0 & \text{if } 1/\alpha < \gamma < 2 \\ 1 & \text{if } \gamma > 2 \text{ or } \alpha < \min[1/\gamma, 1]. \end{cases} \quad (7)$$

We note that the behavior of g for the special case of $\alpha = 1$ and $\gamma < 1$ cannot be determined by our scaling argument, since both sides of the EG inequalities satisfy the same network-size scalings. To address this problem analytically, it is necessary that we consider the coefficients of the leading N -dependent terms, which is beyond the scope of this Letter. Instead, we settle for its numerical resolution at the end of this Letter.

For the other cases, we can analytically determine the locations of graphicality transitions from Eq. (7). There exist two transition points for each value of α in the range $1/2 < \alpha < 1$, namely the upper transition point $\gamma_U^* = 2$ and the lower transition point $\gamma_L^* = 1/\alpha$. On the other hand, no transition occurs for $0 \leq \alpha \leq 1/2$ where $g = 1$ always holds.

All the predictions on the asymptotic behavior of g can be numerically checked by the evaluation of the EG inequalities. First of all, we can verify all the scalings listed

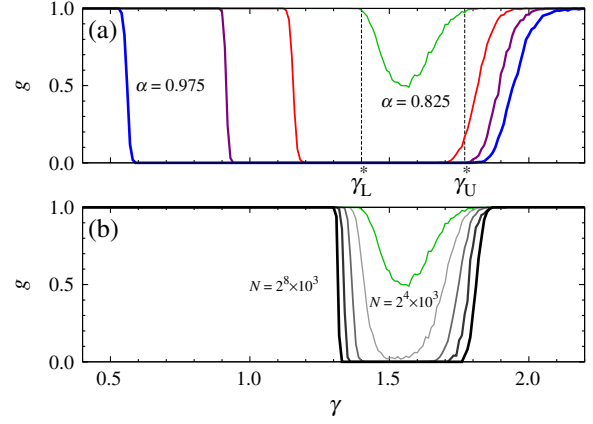


FIG. 2 (color online). γ dependence of the graphicality fraction g obtained from 10^3 random degree sequences. (a) α increases by steps of 0.05 with $N = 2^4 \times 10^3$. γ_L^* and γ_U^* indicate the two transition points at $\alpha = 0.825$, whose N dependence is shown in (b) as N increases by factors of 2.

in Table II, some of which are shown in Fig. 1. This indirectly supports our predictions on the behavior of g , as all the predictions were deduced from those scalings.

To obtain direct support for our predictions, we need to measure the γ dependence of g from the random samples of degree sequences, as illustrated in Fig. 2. Due to sample-to-sample fluctuations at finite system size, g changes continuously between 0 and 1 over a finite range of γ , which becomes narrower as N increases. In fact, g may not even reach 0 if N is too small, as exemplified by the curves for $\alpha = 0.825$ in Fig. 2(a). The curves in Fig. 2(b) show that the minimum of g gradually reaches zero as N increases. Keeping those observations in mind, for the sake of convenience, we regard the range of γ in which g falls below 0.99 as the effectively nongraphical region. Then, the boundary of this region can be chosen as the effective transition points at finite N , which are again marked as γ_L^* and γ_U^* in Fig. 2(a).

We also consider deterministically generated degree sequences defined by $1 - C(k_n) = \nu$, obtained from Eq. (5), which ensures that the sequences exactly follow the network-size scalings of k_n for $n = \nu N$. Those sequences filter out the sample-to-sample fluctuations, making it very straightforward to locate the effective transition points [see the inset Fig. 3(a)]. They also greatly improve the efficiency of calculation, allowing us to check our predictions at larger N . We observe that the transition points estimated by both randomly and deterministically generated degree sequences approach each other as $N \rightarrow \infty$ (for example, see Fig. 4). Therefore, we can use either of those two different samplings to numerically check our predictions.

In Fig. 3, we present graphicality diagrams obtained at two different values of the cutoff coefficient c , where the transition lines at finite network sizes are estimated by the deterministic samplings of degree sequences, and also compared with the transition lines in the thermodynamic

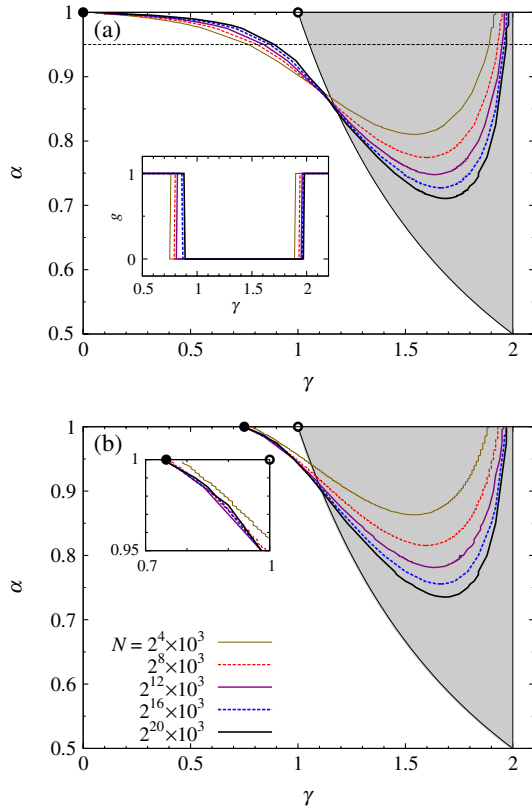


FIG. 3 (color online). Graphicality diagram in the (γ, α) plane at (a) $c = 1$ and (b) $c = 0.6$. The nongraphical region is in gray, while the other lines are the transition lines estimated using deterministic degree sequences, whose behavior of g is as illustrated for $\alpha = 0.95$ in the inset of (a).

limit predicted by the scaling argument. The numerically estimated transition lines tend to approach the analytically predicted ones, which are independent of c . Combining this observation with the verification of the scaling relations listed in Table II, we can safely conclude that the numerical results are slowly converging to our predictions as N increases.

Moreover, Fig. 3 gives us some clues as to the location of the graphicality transition for $\alpha = 1$ and $\gamma < 1$, which could not be determined by the scaling argument as previously explained. The estimated transition lines suggest that the location of the transition is dependent on c : γ_L^* approaches $\gamma = 0$ at $c = 1$, as previously reported [14], but it converges to some different limiting value if $c \neq 1$. The effect of c on the graphicality at $\alpha = 1$ is more closely examined in Fig. 4(a), which suggests that γ_L^* varies continuously between 0 and 1 with c , while γ_U^* converges to 2, regardless of c . This nicely contrasts with Fig. 4(b), which confirms our prediction that the transition points are independent of c for $\alpha < 1$.

While we have given an almost complete picture of the graphicality issue of scale-free networks, the nature of graphicality transitions requires further studies. Note that

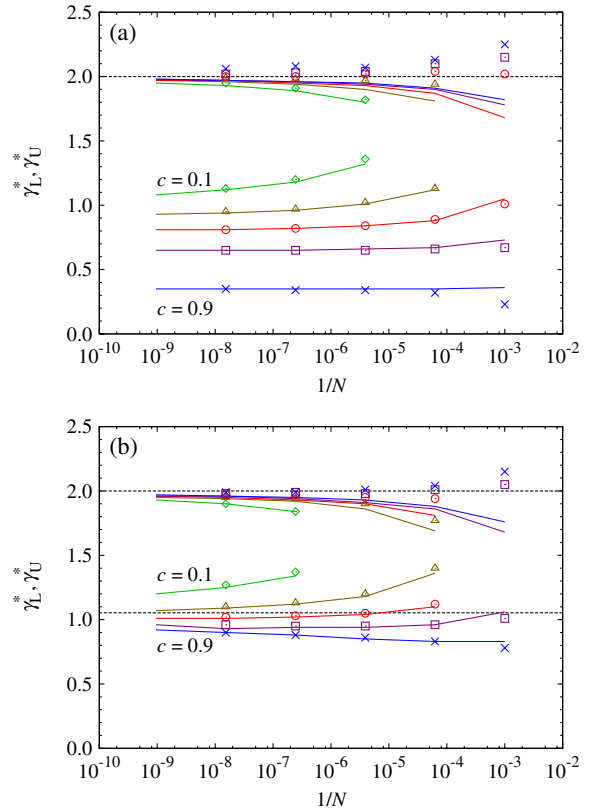


FIG. 4 (color online). N dependence of the transition points as c increases by steps of 0.2 for (a) $k_c = c(N - 1)$ and (b) $k_c = cN^{0.95}$. Symbols indicate the transition points obtained from up to 10^3 random degree sequences, while those obtained from deterministic sequences are connected with lines.

at a transition point, the comparison of scalings fails to determine whether the Erdős-Gallai inequality holds in the asymptotic limit, just like the case of $\alpha = 1$. In such cases, the coefficients of the leading-order terms as well as the second- and higher-order terms must be considered to determine the value of g . Thus, we cannot claim yet that graphicality transitions are truly discontinuous as previously claimed [14], since they might be sharp but continuous transitions resembling the continuous change of γ_L^* with c at $\alpha = 1$. The claim should be either proven or disproven by a more complete understanding of the behavior of g at the transition points.

In conclusion, we have found that in the thermodynamic limit random scale-free networks without self-loops or multiple links are either sparse ($\gamma > 2$) with arbitrary values of degree cutoffs, or dense ($0 < \gamma < 2$) with the upper cutoff $k_c \sim N^\alpha$ satisfying $\alpha < 1/\gamma$, supplementing the statement that “all (random) scale free networks (with maximal range of degree) are sparse.” [14] This also agrees with the upper cutoff found by Seyed-allaei *et al.* [16], which is required for scale-free networks with $\gamma < 2$ generated using a node-fitness mechanism [17]. We also numerically found that the cutoff coefficient c affects the

realizability of degree sequences for the special case of the linear cutoff $\alpha = 1$, which has been overlooked. Our results impose a limit on the values of γ and α for which the properties of random scale-free networks numerically obtained in finite systems can be extrapolated to the thermodynamic limit.

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