

## Asymptotic properties of degree-correlated scale-free networks

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The possible correlation profiles of networks with a given scale-free degree distribution are restricted and bounded by *maximally* correlated configurations. *Dissortative* networks consist of nested bilayers, in which low-degree vertices are connected to high-degree vertices. The number of these bilayers attains a constant value for large network size  $N$ . *Assortative* networks exhibit monolayers of low-degree vertices, the number of which grows monotonously with  $N$ . Analytical relations for the *Pearson* correlation coefficient  $r$  of these extremal configurations are derived and shown to provide lower and upper bounds on the possible  $r$  values. Both bounds are found to vanish for large networks.

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### I. INTRODUCTION

In recent years, many real world systems have been successfully described as complex networks [1–3]. Especially scale-free networks, in which the probability  $P(k)$  of finding a vertex with  $k$  neighbors decays as a power law  $P(k) \sim k^{-\gamma}$  have been studied intensively. Generally, the degree distribution alone does not suffice to completely describe the inner structure of a given network. An important additional measure is given by the so-called assortativity by degree [4,5], which quantifies the tendency of vertices to be connected to other vertices of similar degree. Networks are *assortative* if vertices with high degree preferably connect to other vertices with high degree. Networks are *dissortative* if vertices with high degree are linked to vertices with low degree. Technical and biological networks have been found to be dissortatively mixed, while social networks show assortative correlations (see [2,4,5] for detailed lists).

Degree correlations play an important role for many structural properties of networks, e.g., percolation thresholds [4,6,7], mean distance [6,7], or robustness against vertex removal [4,5,8]. Likewise, they also affect the properties of dynamical processes taking place on networks, such as epidemic spreading [9–11], stability against stimuli and perturbation [12,13], or synchronization of oscillators [14,15].

In this paper, we analyze in detail a class of *maximally* correlated scale-free networks. These networks provide valuable limiting cases for all possible correlation profiles of networks with scale-free degree distributions. We provide an analytical description in terms of the most commonly used measures of assortativity. In particular, we give asymptotic boundary values for the range of all possible values of the *Pearson* correlation coefficient, which is found to vanish for large networks.

Further, we give an intuitive characterization of maximally correlated networks in terms of layers of vertices of the same degree. We find a pronounced community structure that can be useful for the understanding of various phenomena taking place on scale-free networks.

Our paper is organized as follows: in Sec. II, we introduce the basic parameters of our system, discuss the different measures of assortativity, and review the algorithm from [6,7] that we use to construct maximally correlated networks.

We then analyze the structural properties of (i) maximally dissortative and (ii) maximally assortative networks before we close with a brief discussion and summary.

### II. MODELS AND METHODS

We use scale-free networks with a fixed degree distribution given by

$$P(k) = \frac{1}{\mathcal{A}} k^{-\gamma} \quad \text{for } k_0 \leq k \leq k_{\max}$$

$$= 0 \quad \text{otherwise,} \quad (1)$$

where  $\mathcal{A}$  denotes the normalization constant. The structural parameters of our networks are the number of vertices  $N$ , the exponent  $\gamma$ , and the minimal degree  $k_0$ . In this work, we focus on the range  $2 < \gamma < 3$ , which applies to most real world networks. Further, we consider only simple networks without multiple connections or self-loops [29]. For the maximal degree  $k_{\max}$ , we use the so-called *natural* cutoff [16]

$$k_{\max} = k_0 N^{1/(\gamma-1)}. \quad (2)$$

A combination of the two relations (1) and (2) leads to the normalization constant

$$\mathcal{A} = \sum_{k=k_0}^{k_{\max}} k^{-\gamma} \approx \int_{k_0}^{k_{\max}} k^{-\gamma} dk = \frac{1}{\gamma-1} k_0^{1-\gamma} \left(1 - \frac{1}{N}\right). \quad (3)$$

Depending on the parameters  $\gamma$  and  $k_0$ , there is a certain network size, below which  $k_{\max}$  exceeds  $N$ . In the latter case, we use  $k_{\max} = N - 1$ , so that the maximal degree can be written as

$$k_{\max} = \min(k_0 N^{1/(\gamma-1)}, N - 1) \quad (4)$$

for all values of  $N$ . The natural cutoff follows from the well-known configuration model [17] that we use to generate the networks for our simulations. Many structural properties of scale-free networks depend on the scaling of  $k_{\max}$  with  $N$ , such as the probability of multiple links and self-loops [18] or clustering [19]. As discussed in detail in [18,20,21], the cutoff also plays an important role for the construction of scale-free networks with a given correlation profile. As men-

tioned before, we consider the opposite case: We take the degree distribution as fixed and study the subsequent constraints on the *maximal* degree correlations. The qualitative results presented below do not depend on the choice of the maximal degree, while the analytical calculations can easily be adapted to other choices of  $k_{\max}$ .

**A. Measures of assortativity**

A complete description of the degree correlations within a network is provided by the joint probability  $P(j, k)$  that a randomly chosen link connects two vertices of degree  $j$  and  $k$ . This quantity has been used in [22,23] to study the correlations in protein interaction networks and the internet. The interpretation of  $P(j, k)$  is often difficult because of large statistical fluctuations that occur especially for high degrees. As a more robust measure the average degree

$$K_{\text{nn}}(k) \equiv \sum_j jP(j|k) \tag{5}$$

of the neighbors of a randomly chosen vertex of degree  $k$  was introduced in [24,25], where  $P(j|k)$  denotes the conditional probability that the neighbor of a vertex with degree  $k$  has degree  $j$ . The conditional probability  $P(j|k)$  is related to the joint probability  $P(j, k)$  via

$$P(j|k) = \frac{P(j, k)}{P_M(k)}, \tag{6}$$

where  $P_M(k)$  is the probability to find a vertex of degree  $k$  at the end of a randomly chosen edge with

$$P_M(k) = \frac{P(k)k}{\sum_{k'=k_0}^{k_{\max}} P(k')k'} = \frac{P(k)k}{\langle k \rangle_N}. \tag{7}$$

Here and below, the index  $N$  of  $\langle \cdot \rangle_N$  indicates an average over all  $N$  vertices. In *uncorrelated* networks, the degrees of two neighboring vertices are statistically independent, so the joint probability factorizes as  $P^u(j, k) = P_M(j)P_M(k)$  and  $P(j|k)$  is identical to the probability  $P_M(j)$ . Inserting Eq. (7) in Eq. (5) leads to

$$K_{\text{nn}}^u(k) \equiv K_{\text{nn}}^u \equiv \sum_j \frac{jjP(j)}{\langle k \rangle_N} = \frac{\langle k^2 \rangle_N}{\langle k \rangle_N}, \tag{8}$$

i.e.,  $K_{\text{nn}}$  does not depend on  $k$  in networks without degree correlations. Assortatively mixed networks are associated with an increase in  $K_{\text{nn}}$  as a function of  $k$ , while dissortative networks show a decrease in  $K_{\text{nn}}$  as  $k$  increases.

An even more compact and widely used measure for assortativity has been introduced in [4,5]. The assortativity of a given network is measured by a single scalar parameter  $r$  that is basically the *Pearson* correlation coefficient

$$r \equiv \frac{\sum_{j,k} jk[P(j, k) - P_M(j)P_M(k)]}{\sigma_{M,j}\sigma_{M,k}}. \tag{9}$$

for the degrees  $j$  and  $k$  of the two vertices on both ends of a randomly chosen edge [30]. The correlation coefficient is

normalized by the standard deviations  $\sigma_{M,j} \equiv \sqrt{\langle j^2 \rangle_M - \langle j \rangle_M^2}$  and  $\sigma_{M,k} \equiv \sqrt{\langle k^2 \rangle_M - \langle k \rangle_M^2}$ , such that its value lies in the range  $-1 \leq r \leq 1$ . Note that the index  $M$  of  $\langle \cdot \rangle_M$  indicates an average over all  $M$  edges in the network. From Eq. (9) it is easy to see that uncorrelated networks, with  $P(j, k) = P^u(j, k) = P_M(j)P_M(k)$  are characterized by a vanishing correlation coefficient  $r=0$ . A positive correlation coefficient  $r > 0$  indicates assortative mixing, negative values likewise dissortative correlations. However, as we will show below, this distinction can be misleading for networks with broad degree distributions and should be checked carefully.

**B. Rewiring procedure for maximal correlations**

There is a variety of algorithms available in order to construct correlated networks. In Refs. [5,21,26], different methods are introduced, for which both the degree distribution *and* the correlation structure are given. Such algorithms are especially useful for the analysis of real world networks, where null models are needed that conserve certain statistical properties, but are otherwise as uncorrelated as possible. In this paper, we follow a somewhat complementary approach. We study the constraints that a prescribed degree distribution of a network poses on its possible degree correlations. We therefore use a rewiring algorithm from Refs. [6,7] that allows for the construction of maximally correlated configurations for a given network with fixed degree sequence. In each step of the iterative algorithm, two edges with four vertices at their ends are chosen at random. Now, we label these vertices with  $a, b, c$ , and  $d$  such that their degrees  $k_a, k_b, k_c$ , and  $k_d$  are ordered as

$$k_a \geq k_b \geq k_c \geq k_d. \tag{10}$$

Breaking of the two edges and rewiring of the vertices to form pairs  $a, b$  and  $c, d$  leads to assortative networks, while connecting  $a$  with  $d$  and  $b$  with  $c$  leads to dissortative networks. For simple networks, we check during an additional step, whether the new connections are allowed and return to the previous configuration otherwise.

The networks that are obtained after iteration of this procedure are maximally assortative or dissortative both in an intuitive fashion as well as in the sense that the *Pearson* coefficient attains its maximal or minimal value  $r_{\max}$  or  $r_{\min}$ , respectively. To show this, we rewrite definition (9) of  $r$  as

$$r = \frac{\langle jk \rangle_M - \langle j \rangle_M \langle k \rangle_M}{\sigma_{M,j}\sigma_{M,k}} \tag{11}$$

$$= \frac{\sum_{m=1}^M j_m k_m - \frac{1}{M} \left( \sum_{m=1}^M k_m \right)^2}{\sum_{m=1}^M k_m^2 - \frac{1}{M} \left( \sum_{m=1}^M k_m \right)^2}. \tag{12}$$

From degree distribution (1) we know that there are  $NP(k)$  vertices of degree  $k$  in the network and hence  $NP(k)k$  edges emerging from them. Therefore, we can express the sums over all  $M$  links in Eq. (12) as sums over all degrees and obtain

$$\sum_{m=1}^M k_m = \sum_{k=k_0}^{k_{\max}} NP(k)k^2 = N\langle k^2 \rangle_N, \quad (13)$$

$$\sum_{m=1}^M k_m^2 = \sum_{k=k_0}^{k_{\max}} NP(k)k^3 = N\langle k^3 \rangle_N. \quad (14)$$

Using Eqs. (13) and (14), we can rewrite  $r$  in Eq. (12) in terms of the moments of the degree distribution, which leads to

$$r \equiv \frac{A_r - B_r}{C_r - B_r}, \quad (15)$$

with

$$A_r \equiv \sum_{m=1}^M j_m k_m, \quad (16)$$

$$B_r \equiv \frac{N^2}{M} \langle k^2 \rangle_N^2, \quad (17)$$

and

$$C_r \equiv N\langle k^3 \rangle_N. \quad (18)$$

Since the degree distribution  $P(k)$  is fixed, both  $B_r$  and  $C_r$  are fixed as well and do not change as one rewires the network. The only term that is affected by this rewiring is  $A_r$ , as given by Eq. (16), which enters the numerator of Eq. (15). There are only three possibilities to distribute two edges between four vertices, which lead to the terms

$$k_a k_b + k_c k_d, \quad (19)$$

$$k_a k_d + k_b k_c, \quad (20)$$

$$k_a k_c + k_b k_d \quad (21)$$

in  $A_r$ . These terms satisfy the relations

$$k_a k_d + k_b k_c = k_a k_c + k_b k_d - (k_a - k_b)(k_c - k_d), \quad (22)$$

$$k_a k_c + k_b k_d = k_a k_b + k_c k_d - (k_a - k_d)(k_b - k_c). \quad (23)$$

It now follows from these two relations together with Eq. (10) that

$$k_a k_d + k_b k_c \leq k_a k_c + k_b k_d \leq k_a k_b + k_c k_d. \quad (24)$$

Therefore, configuration (19) gives the biggest and configuration (20) the smallest contribution to  $A_r$  and, thus, to  $r$ . These are exactly the chosen configurations in the two versions of the algorithm, so successive iteration of these choices will eventually lead to an asymptotic network with maximal degree correlations, where  $r$  attains its maximal and minimal values  $r_{\max}$  and  $r_{\min}$  respectively. In general, it is possible that such a simple ‘‘hill climbing’’ algorithm becomes trapped in local minima. We therefore checked very carefully that this is not the case in this system. First, we performed several realizations of the random search path starting from the same initial network, each with  $\mathcal{O}(M^2)$  it-

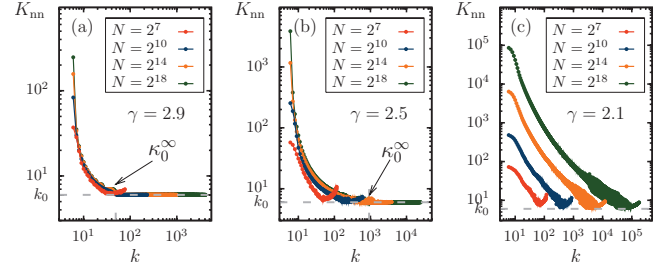


FIG. 1. (Color) Average degree  $K_{nn}$  of the nearest neighbors of a randomly picked vertex with degree  $k$  for maximally dissortative networks with different sizes  $N$  and exponent (a)  $\gamma=2.9$ , (b)  $\gamma=2.5$ , and (c)  $\gamma=2.1$ . All curves are averages over 100 networks with  $k_0=6$ . Sufficiently large networks in (a) and (b) show a plateau with  $k \geq \kappa_0$  for which  $K_{nn}(k)=k_0$ . The asymptotic values  $\kappa_0^\infty$  as given by Eq. (32) are indicated by the arrows.

eration steps. When we compare the resulting networks, we find that all properties discussed below are preserved across all final network configurations. Second, in analogy with simulated annealing, i.e., with increasing the temperature in order to overcome local energy barriers, we allowed for random rewiring with a certain probability  $p$  in each iteration step. Starting from completely random rewiring with  $p=1$  and decreasing the ‘‘temperature’’ stepwise to  $p=0$ , we again converge to the same final configurations as before.

In the following sections, we will analyze the structure of such networks in detail and give analytical expressions for  $r_{\min}$  and  $r_{\max}$ . We begin with a discussion of maximally dissortative networks.

### III. MAXIMALLY DISSORTATIVE NETWORKS

#### A. Structural properties

Figure 1 shows the average nearest-neighbor degree  $K_{nn}(k)$  for maximally dissortative networks for different network sizes  $N$  and decay exponent  $\gamma$ . All curves exhibit the expected decrease of  $K_{nn}$  with increasing  $k$ , only for large  $k$  some curves show a small increase in  $K_{nn}(k)$ . The respective vertices have so many edges that they cannot be saturated with low-degree vertices alone so that they connect also to some vertices with a higher degree. This effect is more pronounced for networks with small  $N$  and small exponent  $\gamma$ . For sufficiently large  $N$  and  $\gamma$ , we find the high-degree region  $k \geq \kappa_0$  for which  $K_{nn}(k)=k_0$ , i.e., all vertices with degree  $k \geq \kappa_0$  are predominantly connected to  $k_0$  vertices. Close inspection of Figs. 1(a) and 1(b) reveals that for large networks the value of  $\kappa_0$  does not depend on  $N$ .

For a more detailed analysis of the structure of these networks, we consider the adjacency matrix  $\mathbf{A}$ , which has  $N \times N$  entries  $A_{ij}$  with  $A_{ij}=1$  if the vertices  $i$  and  $j$  are connected and  $A_{ij}=0$  otherwise. When the indices are rearranged according to the degree of the vertices, one can clearly identify distinct rectangular patterns of connected vertices (see Fig. 2). These patterns correspond to nested bilayers, where vertices with low degree are connected to vertices with high degree. Since the adjacency matrix is symmetric with  $A_{ji}=A_{ij}$ , the ‘‘necklace’’ contains a central cluster with degree

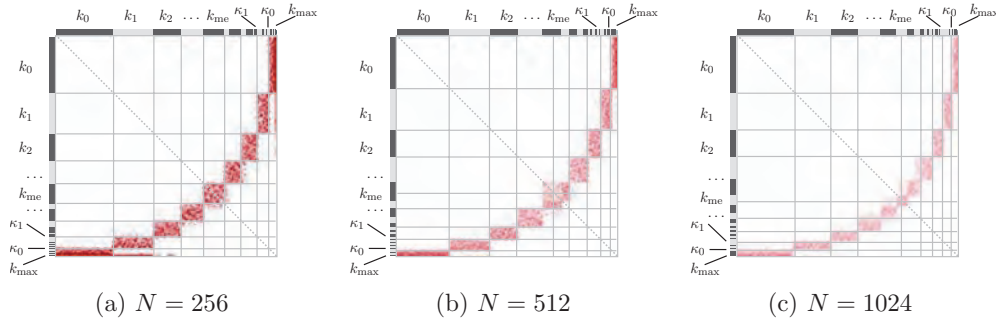


FIG. 2. (Color) Adjacency matrix  $\mathbf{A}$  for three maximally dissortative networks with  $\gamma=2.9$ ,  $k_0=6$  and different sizes (a)  $N=256$ , (b)  $N=512$ , and (c)  $N=1024$ . The vertices are arranged according to their degree, starting with the  $k_0$  vertices at the upper left corner to the  $k_{\max}$  vertex, whose connections are displayed in the last row and column. Red dots represent nonzero matrix elements  $A_{ij}=1$ . Since  $A_{ij}=A_{ji}$  the diagrams are symmetric with respect to the dashed diagonals. The bars at the top and on the left of each matrix provide a guide to the eye by highlighting groups of vertices with identical degree by the same color. All network sizes in (a)–(c) show pronounced rectangular regions that correspond to bilayers of vertices.

$k_{\text{me}}$ . On the low-degree side, the vertices are characterized by a single degree  $k_n < k_{\text{me}}$ , the vertices on the high-degree side have degrees in between the boundary values  $\kappa_n \leq k \leq \kappa_{n-1}$ . The outermost bilayer consists of the  $k_0$  vertices that connect to all vertices with  $\kappa_0 \leq k \leq k_{\max}$ , which leads to the region of  $K_{\text{m}}(k \geq \kappa_0) \approx k_0$  that can be identified in Fig. 1. The second bilayer contains all vertices with  $k_0+1$  on the one side and all vertices with  $\kappa_1 \leq k \leq \kappa_0$  on the other side, the third one all vertices with  $k_0+2$  and  $\kappa_2 \leq k \leq \kappa_1$ , and so forth. The total number of bilayers is limited by the central cluster of  $k_{\text{me}}$  vertices, around which they are nested (see Fig. 2). Note that in principle, network realizations might be generated, in which some of the bilayers disconnect completely from the rest of the network. However, in practice, in our simulations we find that the corresponding degree sequences, for which the numbers of edges on both sides of a bilayer match *exactly*, are extremely unlikely to occur [31].

In addition to the necklace of clusters, we find for small networks as in Figs. 2(a) and 2(b) that the last row and column, which represent the  $k_{\max}$  vertices, are connected to several low-degree layers, corresponding to the increase in  $K_{\text{m}}$  for large degrees in Fig. 1.

In the following, we will consider these effects in more detail and begin with the influence of the  $k_{\max}$  vertex. It follows from the expression in Eq. (4) that the upper cutoff is given by  $k_{\max}=N-1$  for

$$N < N_1 \equiv k_0^{(\gamma-1)/(\gamma-2)}, \quad (25)$$

so vertices with degree  $k_{\max}$  are connected to all remaining vertices in the network. For  $N > N_1$ , the  $k_{\max}$  vertex no longer spans the entire network but is still connected to all vertices with  $k_0 \leq k \leq k_A$ . The value of  $k_A$  can be determined from the relation

$$k_{\max} = \sum_{k=k_0}^{k_A} N_k \approx \int_{k_0}^{k_A} NP(k)dk = \frac{1}{1-\gamma} \frac{N}{\mathcal{A}} (k_A^{1-\gamma} - k_0^{1-\gamma}), \quad (26)$$

where  $N_k$  denotes the number of vertices with degree  $k$ . Solving Eq. (26) for  $k_A$  leads to

$$k_A = k_0 \left[ 1 - \left( 1 - \frac{1}{N} \right) k_0 N^{(2-\gamma)/(\gamma-1)} \right]^{1/(1-\gamma)}. \quad (27)$$

For  $N=256$ ,  $\gamma=2.9$ , and  $k_0=6$ , relation (27) gives  $k_A \approx 8$ , which agrees well with Fig. 2(a), where the  $k_{\max}$  vertex protrudes into the layer of  $k=8$ . In the limit of large networks with  $N \gg N_1$ , expression (27) behaves as  $k_A \approx k_0$ , and all edges of the  $k_{\max}$  vertex are saturated by  $k_0$  vertices [see Fig. 2(c)]. As we have seen above, the  $k_0$  vertices are numerous enough to saturate all vertices with degree  $k \geq \kappa_0$ , which leads to the formation of the outermost bilayer. The value of  $\kappa_0$  can be obtained from

$$N_{k_0} k_0 = \sum_{k=\kappa_0}^{k_{\max}} N_k k, \quad (28)$$

or

$$\begin{aligned} NP(k_0)k_0 &= \sum_{k=\kappa_0}^{k_{\max}} NP(k)k \approx \int_{\kappa_0}^{k_{\max}} NP(k)k dk \\ &= \frac{1}{2-\gamma} \frac{N}{\mathcal{A}} (k_{\max}^{2-\gamma} - \kappa_0^{2-\gamma}). \end{aligned} \quad (29)$$

Solving Eq. (29) for  $\kappa_0$  leads to

$$\kappa_0 = k_0 \left( \frac{\gamma-2}{k_0} + N^{(2-\gamma)/(\gamma-1)} \right)^{1/(2-\gamma)}. \quad (30)$$

For large networks with

$$N \gg N_2 \equiv \left( \frac{k_0}{\gamma-2} \right)^{(\gamma-1)/(\gamma-2)}, \quad (31)$$

the degree  $\kappa_0$  attains the constant value

$$\kappa_0 \approx \kappa_0^\infty \equiv k_0^{(\gamma-1)/(\gamma-2)} (\gamma-2)^{1/(2-\gamma)}. \quad (32)$$

This behavior can be seen in Figs. 1(a) and 1(b), where the values of  $\kappa_0^\infty$  as obtained from Eq. (32) are indicated. For  $\gamma=2.1$  as in Fig. 1(c) the value of  $N_2$  as defined by Eq. (31) is given by  $N_2 \approx 3.6 \times 10^{19} > 2^{64}$ , so the depicted network sizes are too small to observe the plateau behavior.



Using expression (32) for  $\kappa_0$ , we can also determine the values of the degrees  $\kappa_n$  that determine the borders of the large degree side of the bilayers. As in Eq. (28), the degree  $\kappa_1$  can be computed by

$$N_{k_0+1}(k_0+1) = \sum_{k=\kappa_1}^{\kappa_0} N_k k, \quad (33)$$

the higher values  $\kappa_2, \kappa_3, \dots$  then follow from iteration of Eq. (33) with the respective limits in the summation. As we have seen in Fig. 2, the series of bilayers is limited by the central degree  $k_{\text{me}}$ . The value of  $k_{\text{me}}$  can be determined using the condition that the number of edges attached to all vertices with  $k < k_{\text{me}}$  is equal to the number of edges attached to all vertices with  $k > k_{\text{me}}$ . Solving the implicit equation

$$\sum_{k=k_0}^{k_{\text{me}}} N_k k = \sum_{k=k_{\text{me}}}^{k_{\text{max}}} N_k k, \quad (34)$$

we obtain

$$k_{\text{me}} = 2^{1/(\gamma-2)} k_0 (1 + N^{(2-\gamma)/(\gamma-1)})^{1/(2-\gamma)}. \quad (35)$$

This expression becomes independent of  $N$  in the limit of large networks and attains the asymptotic value

$$k_{\text{me}} \approx k_{\text{me}}^\infty \equiv 2^{1/(\gamma-2)} k_0. \quad (36)$$

The number  $N_{\text{bi}}$  of bilayers as given by  $k_{\text{me}} - k_0$  is therefore limited and reaches

$$N_{\text{bi}} \leq \max(N_{\text{bi}}) = k_{\text{me}}^\infty - k_0 \quad (37)$$

for large networks.

### B. Scaling relation for $r_{\text{min}}$

After the detailed description of the layered structure of maximally assortative networks, we will now discuss asymptotic estimates for the corresponding minimal assortativity coefficient  $r = r_{\text{min}}$ . We start from the general expression as given by Eq. (15). As we have seen before, the only term that depends on the degree correlation is  $A_r$  as given by Eq. (16); minimal assortativity  $r_{\text{min}}$  can therefore be expressed as

$$r_{\text{min}} = \frac{\min(A_r) - B_r}{C_r - B_r}. \quad (38)$$

In the following, we will first determine the asymptotic behavior of  $B_r$  and  $C_r$  as given by Eqs. (17) and (18) and then address the scaling behavior of  $\min(A_r)$ . We start with the total number of edges  $M$ , which can be obtained from

$$\begin{aligned} M = N \langle k \rangle_N &= N \sum_{k=k_0}^{k_{\text{max}}} P(k) k = \frac{N}{\mathcal{A}} \sum_{k=k_0}^{k_{\text{max}}} k^{1-\gamma} \approx \frac{N}{\mathcal{A}} \int_{k_0}^{k_{\text{max}}} k^{1-\gamma} dk \\ &= \frac{\gamma-1}{\gamma-2} N k_0 \frac{1 - N^{(2-\gamma)/(\gamma-1)}}{1 - \frac{1}{N}}. \end{aligned} \quad (39)$$

The moments of degree distribution (1) have the general form

$$\begin{aligned} \langle k^n \rangle_N &= \sum_{k=k_0}^{k_{\text{max}}} P(k) k^n \approx \int_{k_0}^{k_{\text{max}}} P(k) k^n dk \\ &= k_0^n \frac{\gamma-1}{n+1-\gamma} \frac{1}{1 - \frac{1}{N}} (N^{(n+1-\gamma)/(\gamma-1)} - 1). \end{aligned} \quad (40)$$

It now follows from expressions (39) and (40) for the total edge number  $M$  and the second moment  $\langle k^2 \rangle_N$  that the term  $B_r$  as defined in Eq. (17) scales as

$$B_r \sim k_0^3 N^{3/(\gamma-1)} \quad \text{for } 1 < \gamma < 2 \quad (41)$$

$$\sim k_0^3 N^{(5-\gamma)/(\gamma-1)} \quad \text{for } 2 < \gamma < 3 \quad (42)$$

$$\sim k_0^3 N \quad \text{for } 3 < \gamma \quad (43)$$

in the limit of large  $N$ . Likewise, the large- $N$  behavior of the term  $C_r$  is given by

$$C_r \sim k_0^3 N^{3/(\gamma-1)} \quad \text{for } 1 < \gamma < 4 \quad (44)$$

$$\sim k_0^3 N \quad \text{for } 4 < \gamma, \quad (45)$$

as follows from expression (40) for the third moment  $\langle k^3 \rangle_N$ .

Finally, we now derive the scaling behavior of  $\min(A_r)$ . In order to do so, it is convenient to assign an arbitrary but fixed direction to each edge  $m$ , such that it emanates from a vertex with degree  $j_m$  and points at a vertex with degree  $k_m$ . Now we label the edges in such a way that the degrees of the vertices they point at increase, i.e.,

$$k_1 \leq k_2 \leq \dots \leq k_M. \quad (46)$$

In assortative networks, low-degree vertices are connected to high-degree vertices. The smallest value of  $A_r$  is then obtained in a configuration, where the degrees of the vertices, from which the edges in Eq. (46) emanate, decrease. This corresponds to

$$j_m = J_m \equiv k_{M-m} \quad (47)$$

so that the sequence of  $J_1, J_2, \dots, J_M$  satisfies accordingly

$$J_1 \geq J_2 \geq \dots \geq J_M. \quad (48)$$

When self- and multiple connections are allowed, it is always possible to rewire a given network such that Eqs. (46)–(48) are fulfilled. However, in assortatively mixed networks multiple edges do not play an important role anyway, because these networks contain many vertices with small degrees that can be connected to the few hubs, and multiple connections can therefore be avoided. In the limit of large networks, the fraction of multiple edges vanishes, so we can use Eqs. (46)–(48) also for simple networks. The choice in Eq. (47) leads to

$$\min(A_r) = \sum_{m=1}^M k_m J_m = \sum_{m=1}^M k_m k_{M-m}. \quad (49)$$

Since the term  $k_m k_{M-m}$  does not change when we substitute  $m$  by  $M-m$ , we also have

$$\min(A_r) = 2 \sum_{m=M/2}^M k_m J_m = 2 \sum_{m=M/2}^M k_m k_{M-m}. \quad (50)$$

From the ordering of the factors  $J_m$  in Eq. (48) we can derive the following inequalities:

$$J_{M/2} = k_{M/2} \geq J_m \geq J_M = k_0 \quad \text{for } M/2 \leq m \leq M. \quad (51)$$

When these inequalities are used in expression (50) for  $\min(A_r)$ , we obtain both an upper and a lower bound for  $\min(A_r)$  as given by

$$2k_{M/2} \sum_{m=M/2}^M k_m \geq \min(A_r) \geq 2k_0 \sum_{m=M/2}^M k_m. \quad (52)$$

By construction, the value of  $k_{M/2}$  is given by the central degree  $k_{\text{me}}$  in Eq. (35), for which the vertices with degree  $k < k_{\text{me}}$  have the same number of edges as the vertices with  $k > k_{\text{me}}$ . For large  $N$ , relation (35) implies the scaling behavior

$$k_{\text{me}} \approx 2^{1/(\gamma-2)} k_0 N^{1/(\gamma-1)} \quad \text{for } 1 < \gamma < 2 \quad (53)$$

$$\approx 2^{1/(\gamma-2)} k_0 \quad \text{for } 2 < \gamma. \quad (54)$$

The sum over  $M/2$  edges in Eq. (52) can again be transformed into a sum over all degrees,

$$\begin{aligned} \sum_{m=M/2}^M k_m &= \sum_{k=k_{\text{me}}}^{k_{\text{max}}} NP(k)k^2 \approx \int_{k_{\text{me}}}^{k_{\text{max}}} NP(k)k^2 dk \\ &= \frac{N}{\mathcal{A}} \frac{1}{3-\gamma} (k_{\text{max}}^{3-\gamma} - k_{\text{me}}^{3-\gamma}), \end{aligned} \quad (55)$$

together with the asymptotic behavior of  $k_{\text{me}}$  in Eq. (54) we find

$$\sum_{m=M/2}^M k_m \sim k_0^2 N^{2/(\gamma-1)} \quad \text{for } 1 < \gamma < 3 \quad (56)$$

$$\sim k_0 N \quad \text{for } 3 < \gamma. \quad (57)$$

We now combine the asymptotic behavior of  $k_{\text{me}}$  and  $\sum_{m=M/2}^M k_m$  as given by Eqs. (53), (54), (56), and (57) with the two inequalities contained in Eq. (52). First, we insert Eqs. (53) and (56) into Eq. (52) and obtain

$$c_1 k_0^3 N^{3/(\gamma-1)} \geq \min(A_r) \geq c_2 k_0^3 N^{2/(\gamma-1)} \quad (58)$$

for  $1 < \gamma < 2$  with two  $\gamma$ -dependent constants  $c_1$  and  $c_2$ . This implies the asymptotic behavior of  $\min(A_r)$  as given by

$$\min(A_r) \sim k_0^3 N^\zeta \quad \text{for } 1 < \gamma < 2 \quad (59)$$

for large  $N$  where the exponent  $\zeta$  satisfies the inequalities

$$\frac{2}{\gamma-1} \leq \zeta \leq \frac{3}{\gamma-1}. \quad (60)$$

Second, we use the asymptotic behavior in Eqs. (54) and (56) together with the inequalities (52) to obtain

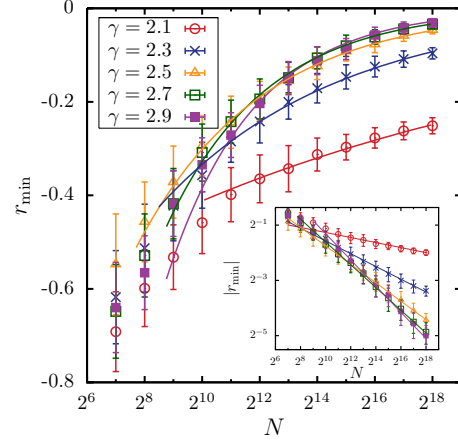


FIG. 3. (Color online) *Pearson* coefficient  $r_{\text{min}}$  for maximally dissortative networks as a function of network size  $N$  for different values of the scaling exponent  $\gamma$ . All data points are averages over 100 networks with minimal degree  $k_0=6$ , error bars denote the standard deviation. The lines are fits using Eq. (64) with the amplitude as the only fit parameter. For all values of the exponent  $\gamma$ , the data for the minimal *Pearson* coefficient  $r_{\text{min}}$  decay to zero for large  $N$ , in good agreement with the theoretical predictions. The inset shows the same data for  $|r_{\text{min}}|$  as a function of  $N$  in a double-logarithmic plot. All curves clearly exhibit the expected power-law scaling as in Eq. (64).

$$c_1' k_0^3 N^{2/(\gamma-1)} \geq \min(A_r) \geq c_2' k_0^3 N^{2/(\gamma-1)} \quad (61)$$

for  $2 < \gamma < 3$ , which leads to

$$\min(A_r) \sim k_0^3 N^{2/(\gamma-1)} \quad \text{for } 2 < \gamma < 3. \quad (62)$$

For the region  $\gamma > 3$ , we combine the two asymptotic relations (54) and (57) with the inequalities (52) and obtain

$$\min(A_r) \sim k_0^3 N \quad \text{for } 3 < \gamma. \quad (63)$$

Putting the relations for  $\min(A_r)$  as given by Eqs. (59)–(63) together with  $B_r$  and  $C_r$  in Eqs. (41)–(45) we finally arrive at a general expression for the scaling behavior of the *Pearson* coefficient for maximally dissortative networks:

$$\begin{aligned} r_{\text{min}} &\sim -c_1(\gamma, k_0) \quad \text{for } \gamma < 2 \\ &\sim -N^{(2-\gamma)/(\gamma-1)} \quad \text{for } 2 < \gamma < 3 \\ &\sim -N^{(\gamma-4)/(\gamma-1)} \quad \text{for } 3 < \gamma < 4 \\ &\sim -c_2(\gamma, k_0) \quad \text{for } 4 < \gamma, \end{aligned} \quad (64)$$

with the two  $\gamma$ - and  $k_0$ -dependent constants  $c_1$  and  $c_2$ . For  $2 < \gamma < 3$  the same result has also been derived in [27].

For  $2 < \gamma < 4$  it follows from Eq. (64) that the correlation coefficient vanishes in the limit of large  $N$ , which is confirmed by simulations (see Fig. 3). This is surprising since the structure of the underlying networks is nevertheless highly correlated, as we have seen in the previous section. We conclude that while uncorrelated networks are characterized by a vanishing correlation coefficient, the opposite is not necessarily true. Especially for large networks, the *Pearson* coefficient is not sufficient to judge the correlation

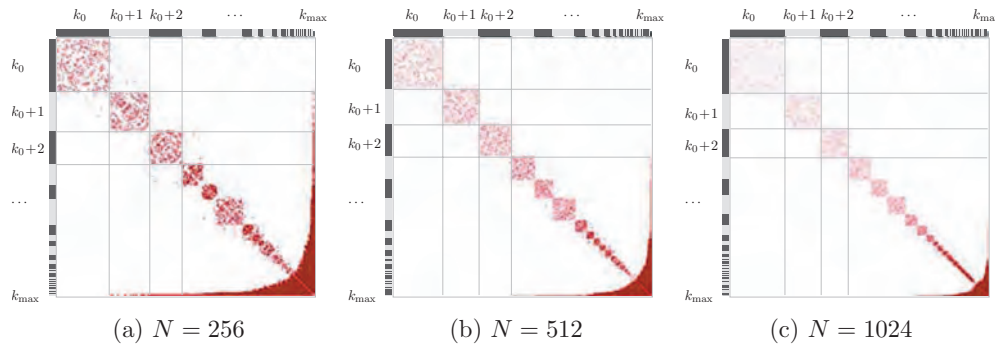


FIG. 4. (Color) Adjacency matrix  $\mathbf{A}$  for three maximally assortative networks with  $\gamma=2.5$ ,  $k_0=6$  and different sizes (a)  $N=256$ , (b)  $N=512$ , and (c)  $N=1024$ . As in Fig. 2, the entries are ordered according to the degree of the vertices. The bars on top and on the right of each panel correspond to groups of vertices that have the same degree. Red dots indicate nonzero matrix elements  $A_{ij}=A_{ji}=1$ . In (a)–(c) we find an increasing number of pronounced layers of vertices that are connected to vertices with the same degree. The number of such layers is limited by the large degree vertices that form a region in the lower right corner that spans several layers.

structure of a given network, and additional measures need to be taken into account.

#### IV. MAXIMALLY ASSORTATIVE NETWORKS

We will now turn to maximally *assortative* networks, starting with a discussion of their main structural characteristics.

##### A. Structural properties

For a first overview, we consider again the adjacency matrix  $\mathbf{A}$  (see Fig. 4). Using the previously explained ordering according to the degree of the vertices, we find pronounced quadratic regions in  $\mathbf{A}$ . These regions represent monolayers of vertices, which are only connected to vertices of the same degree. A comparison of Figs. 4(a)–4(c) shows that the number of such layers grows with network size  $N$ . Furthermore, inspection of these figures also reveals a region of high-degree vertices with  $k \lesssim k_{\max}$ , the edges of which span several layers of vertices and thereby limit the number of low-degree vertices that are connected only to vertices of the same degree. The relative size of this region of high-degree vertices in the lower right corner in Figs. 4(a)–4(c) decreases with increasing network size  $N$ .

For a more detailed analysis, we consider again the average nearest-neighbor degree  $K_{\text{nn}}(k)$  in Fig. 5 for networks with different sizes  $N$  and exponent  $\gamma$ . Most curves exhibit a region of low degrees  $k \leq k_s$ , for which  $K_{\text{nn}}(k) \approx k$ . This corresponds to the described layers of vertices that saturate all their edges with vertices of the same degree. We also see that  $k_s$  increases with  $N$ . This region is followed by a region of degrees  $k$  with  $K_{\text{nn}}(k) > k$ . The corresponding vertices are not only connected to vertices with the same degree, but additionally to vertices of higher degree. As we have seen in Fig. 4, these edges emerge from high-degree vertices that are not numerous enough in order to saturate all their edges with vertices of the same degree. Subsequently, they have to “export” some of their edges to vertices with smaller  $k$ . All depicted networks in Fig. 5 show therefore a *dissortative* region for large  $k$ , where  $K_{\text{nn}}$  decreases with growing  $k$ ,

although the networks are maximally assortative. This effect is more pronounced for smaller values of  $\gamma$ . None of the networks with  $\gamma=2.1$  in panel (c) exhibits a region of small  $k$ , where vertices are only connected among themselves. In the following, we will state the qualitative observations more precisely by analytical considerations.

Scale-free networks are characterized on one hand by a large number of low-degree vertices that could in principal form regular subgraphs, where all vertices have the same degree. On the other hand, there are few vertices with very large degrees that cannot saturate all their edges only among themselves. In between lies some degree  $\hat{k}$ , where the number of vertices  $N_{\hat{k}}$  and the number of respective half edges  $N_{\hat{k}}\hat{k}$  attached to them is exactly sufficient to form a complete graph characterized by

$$\frac{N_{\hat{k}}\hat{k}}{2} = \frac{N_{\hat{k}}(N_{\hat{k}} - 1)}{2}, \quad (65)$$

or

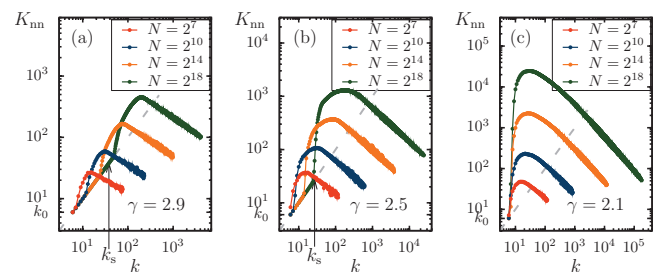


FIG. 5. (Color) Average degree  $K_{\text{nn}}$  of the nearest neighbors of a randomly picked vertex with degree  $k$  for maximally assortative networks for different sizes  $N$  and exponent (a)  $\gamma=2.9$ , (b)  $\gamma=2.5$ , and (c)  $\gamma=2.1$ . All curves are averages over 100 networks with  $k_0=6$ . In (a) and (b) we find for sufficiently large networks a region of small degrees  $k \leq k_s$ , for which  $K_{\text{nn}}(k) \approx k$ . For  $N=2^{18}$  the values of  $k_s$  as given by Eq. (75) are indicated by the arrows. For large  $k$ , all curves show *dissortative* behavior, where  $K_{\text{nn}}$  decreases with increasing  $k$ .

$$\hat{k} = N_{\hat{k}} - 1. \quad (66)$$

Approximating  $N_{\hat{k}} - 1$  by  $N_{\hat{k}} = NP(\hat{k})$  we find from Eq. (66)

$$\hat{k} = \left( \frac{N}{\mathcal{A}} \right)^{1/(\gamma+1)}. \quad (67)$$

Vertices with  $k > \hat{k}$  can connect only  $N_k(N_k - 1)$  edges from their total of  $N_k k$  edges to other vertices of the same degree  $k$ , the rest has to be connected to other vertices with different degrees. For the whole network a total number of  $M_e$  has to be exported in such a fashion,

$$\begin{aligned} M_e &\equiv \sum_{k=\hat{k}}^{k_{\max}} [N_k k - N_k(N_k - 1)] \approx \int_{\hat{k}}^{k_{\max}} [N_k k - N_k(N_k - 1)] dk \\ &= \int_{\hat{k}}^{k_{\max}} \{NP(k)k - NP(k)[NP(k) - 1]\} dk \\ &= \frac{1}{2 - \gamma \mathcal{A}} \left[ \frac{N}{\mathcal{A}} k_0^{2-\gamma} N^{(2-\gamma)/(\gamma-1)} - \left( \frac{N}{\mathcal{A}} \right)^{(2-\gamma)/(\gamma+1)} \right] \\ &\quad - \frac{1}{1 - 2\gamma} \left( \frac{N}{\mathcal{A}} \right)^2 \left[ k_0^{1-2\gamma} N^{(1-2\gamma)/(\gamma-1)} - \left( \frac{N}{\mathcal{A}} \right)^{(1-2\gamma)/(\gamma+1)} \right] \\ &\quad - \frac{1}{1 - \gamma \mathcal{A}} \left[ k_0^{1-\gamma} N^{(1-\gamma)/(\gamma-1)} - \left( \frac{N}{\mathcal{A}} \right)^{(1-\gamma)/(\gamma+1)} \right]. \quad (68) \end{aligned}$$

Taking only the leading terms for large  $N$  into consideration, we obtain for  $\gamma > 2$ ,

$$M_e \approx \left( \frac{1}{\gamma - 2} - \frac{1}{2\gamma - 1} \right) \left( \frac{N}{\mathcal{A}} \right)^{3/(\gamma+1)}. \quad (69)$$

Since these  $M_e$  edges will be connected to vertices with  $k \leq \hat{k}$ , the overall number of edges  $M_s$  that can be connected only between vertices of same degree will be reduced to

$$M_s \equiv M_{k \leq \hat{k}} - M_e, \quad (70)$$

where  $M_{k \leq \hat{k}}$  denotes the number of edges emerging from vertices with  $k \leq \hat{k}$ :

$$\begin{aligned} M_{k \leq \hat{k}} &= \sum_{k=k_0}^{\hat{k}} N_k k \approx \int_{k_0}^{\hat{k}} NP(k)k dk \\ &= \frac{1}{\gamma - 2} \left[ k_0^{2-\gamma} \frac{N}{\mathcal{A}} - \left( \frac{N}{\mathcal{A}} \right)^{3/(\gamma+1)} \right]. \quad (71) \end{aligned}$$

Together with the relation for  $M_e$  in Eq. (69) we obtain for  $M_s$  in Eq. (70)

$$M_s = \frac{k_0^{2-\gamma} N}{\gamma - 2 \mathcal{A}} - \left( \frac{2}{\gamma - 2} - \frac{1}{2\gamma - 1} \right) \left( \frac{N}{\mathcal{A}} \right)^{3/(\gamma+1)}. \quad (72)$$

This expression is in fact negative for network sizes

$$N < N_b \equiv \frac{k_0^2}{\gamma - 1} \left( \frac{3\gamma}{2\gamma - 1} \right)^{(\gamma+1)/(\gamma-2)}, \quad (73)$$

so networks with  $N < N_b$  do not show range of small degrees  $k \leq k_s$ , where vertices are only connected to other vertices of

the same degree. The values obtained from Eq. (73) correspond nicely to our simulation results from Fig. 5: for  $\gamma = 2.9$  we find  $N_b \approx 250$ , and  $N_b \approx 1956$  for  $\gamma = 2.5$ . For  $\gamma = 2.1$  relation (73) evaluates to  $N_b \approx 4.3 \times 10^{10}$ , which is far beyond network sizes that are accessible to computer simulation and explains our findings from Fig. 5(c), where none of the curves shows a region of  $K_{\text{nn}}(k) \approx k$ .

Using  $M_s$  in Eq. (72) we can now give an estimate for the degree  $k_s$ . For the range  $k_0 \leq k \leq k_s$  a total of  $M_s$  edges is available. Solving

$$M_s = \sum_{k=k_0}^{k_s} N_k k \approx \int_{k_0}^{k_s} NP(k)k dk = \frac{N}{\mathcal{A}} \frac{1}{\gamma - 2} (k_0^{2-\gamma} - k_s^{2-\gamma}) \quad (74)$$

for  $k_s$  we obtain

$$k_s = k_0^{(\gamma-1)/(\gamma+1)} (\gamma - 1)^{1/(\gamma+1)} \left( \frac{3\gamma}{2\gamma - 1} \right)^{1/(2-\gamma)} N^{1/(\gamma+1)}. \quad (75)$$

The theoretical values from Eq. (75) agree well with our simulations in Fig. 5, where they are indicated for  $N = 2^{18}$  in panels (a) and (b). Further, relation (75) confirms our observation that the number of low-degree monolayers  $N_{\text{mo}}$  with  $k \leq k_s$  increases with network size  $N$  since

$$N_{\text{mo}} \equiv k_s - k_0 + 1 \sim N^{1/(\gamma+1)}. \quad (76)$$

## B. Scaling relation for $r_{\text{max}}$

In analogy with the case of dissortative networks in Eq. (38), the *Pearson* coefficient attains its maximal value  $r_{\text{max}}$  when

$$r_{\text{max}} = \frac{\max(A_r) - B_r}{C_r - B_r} \quad (77)$$

is fulfilled. Following our considerations about the structure of such networks, we estimate  $\max(A_r)$  through three parts:

$$\max(A_r) = b_1 + b_2 + b_3. \quad (78)$$

The first contribution  $b_1$  is given by the edges within the layers with  $k \leq k_s$ , the second term  $b_2$  consists of the edges that connect vertices with  $k \geq \hat{k}$  to complete subgraphs, and  $b_3$  finally gives the contribution of the exported edges.

We begin with  $b_1$ . In each layer of vertices with degree  $k \leq k_s$  there are  $\frac{1}{2} N_k k$  edges with degrees  $k$  on both of their ends, their contribution to the sum in Eq. (16) is therefore

$$\begin{aligned} b_1 &\equiv \sum_{k=k_0}^{k_s} \frac{1}{2} N_k k k^2 \approx \int_{k_0}^{k_s} \frac{1}{2} NP(k) k^3 dk \\ &= \frac{1}{2(4 - \gamma)} \left( \frac{3\gamma}{2\gamma - 1} \right)^{(4-\gamma)/(2-\gamma)} \left( \frac{N}{\mathcal{A}} \right)^{5/(\gamma+1)} - \frac{k_0^{4-\gamma}}{2(4 - \gamma)} \frac{N}{\mathcal{A}}. \quad (79) \end{aligned}$$

The second contribution is given by  $\frac{1}{2} N_k(N_k - 1)$  edges that form complete graphs of vertices with degree  $k \geq \hat{k}$ ,



$$\begin{aligned}
 b_2 &\equiv \sum_{k=\hat{k}}^{k_{\max}} \frac{1}{2} N_k (N_k - 1) k^2 \approx \sum_{k=\hat{k}}^{k_{\max}} \frac{1}{2} N_k^2 k^2 \\
 &\approx \int_{\hat{k}}^{k_{\max}} \frac{1}{2} [NP(k)]^2 k^2 dk \\
 &= \frac{1}{2(2\gamma-3)} \left[ \left( \frac{N}{\mathcal{A}} \right)^{5/(\gamma+1)} - \frac{k_0^{3-2\gamma}}{\mathcal{A}^2} N^{1/(\gamma-1)} \right]. \quad (80)
 \end{aligned}$$

The third term  $b_3$  compiles the contribution of the  $M_e$  edges that the vertices with  $k > \hat{k}$  cannot saturate between themselves. We estimate their contribution by the assumption that they emerge from vertices with degree  $\hat{k} < k \leq k_{\max}$  and point at vertices degree  $k_s < k \leq \hat{k}$ . The mean degrees of the vertices on the two ends of any edge are then given by  $\langle k_s < k \leq \hat{k} \rangle_M$  and  $\langle \hat{k} < k \leq k_{\max} \rangle_M$ . The contribution of these edges to  $\max(A_r)$  within this rough approximation is then given by

$$b_3 \equiv M_e \langle k_s < k \leq \hat{k} \rangle_M \langle \hat{k} < k \leq k_{\max} \rangle_M. \quad (81)$$

The mean values in Eq. (81) are computed by

$$\langle k_1 < k \leq k_2 \rangle_M \equiv \frac{\int_{k_1}^{k_2} P_M(k) k dk}{\int_{k_1}^{k_2} P_M(k) dk}, \quad (82)$$

with the definition of  $P_M(k)$  from Eq. (7) we find

$$\begin{aligned}
 \langle k_s < k \leq \hat{k} \rangle_M &= \frac{\gamma-2}{3-\gamma} \frac{2\gamma-1}{\gamma+1} \left[ 1 - \left( \frac{3\gamma}{2\gamma-1} \right)^{(3-\gamma)/(2-\gamma)} \right] \\
 &\quad \times \left( \frac{N}{\mathcal{A}} \right)^{1/(\gamma+1)} \quad (83)
 \end{aligned}$$

and

$$\langle \hat{k} < k \leq k_{\max} \rangle_M = \frac{\gamma-2}{3-\gamma} \mathcal{A}^{(2-\gamma)/(\gamma+1)} k_0^{3-\gamma} N^{(5-\gamma)/(\gamma^2-1)}. \quad (84)$$

With Eqs. (83) and (84), together with  $M_e$  from Eq. (69) we can now compute  $b_3$  in Eq. (81) and find

$$\begin{aligned}
 b_3 &= k_0^{3-\gamma} \frac{\gamma-2}{(3-\gamma)^2} \left[ 1 - \left( \frac{2}{3} - \frac{1}{3\gamma} \right)^{(3-\gamma)/(\gamma-2)} \right] \\
 &\quad \times \mathcal{A}^{(-\gamma+2)/(\gamma+1)} N^{(3\gamma+1)/(\gamma^2-1)}. \quad (85)
 \end{aligned}$$

Combining the three terms from Eqs. (79), (80), and (85) yields the following scaling behavior of  $\max(A_r)$  in Eq. (78) for large network sizes  $N$ :

$$\max(A_r) \approx \alpha N^{5/(\gamma+1)} + \beta N^{5/(\gamma+1)} + \delta N^{(3\gamma+1)/(\gamma^2-1)}, \quad (86)$$

where  $\alpha$ ,  $\beta$ , and  $\delta$  are constants depending on  $\gamma$  and  $k_0$ . A comparison of the contributions leads to

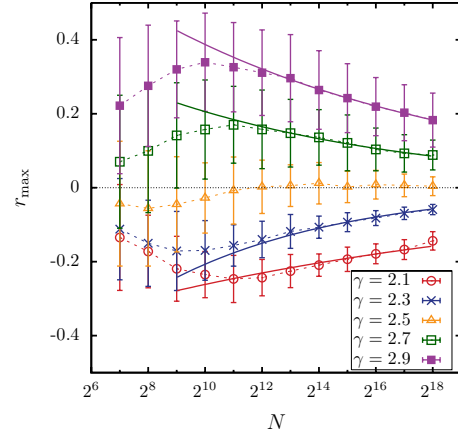


FIG. 6. (Color online) *Pearson* coefficient  $r_{\max}$  for maximally assortative networks as a function of network size  $N$  for different values of the scaling exponent  $\gamma$ . All data points are averages over 100 networks with minimal degree  $k_0=6$ , error bars denote the standard deviation. The continuous lines are fits as obtained from the relations in Eq. (88) with the amplitude as the only fit parameter. The dashed lines connect the data points to guide the eye. In agreement with the theoretical results, the *Pearson* coefficient  $r_{\max}$  is negative for networks with  $\gamma < 2.5$  and goes to zero for large  $N$ .

$$\max(A_r) \sim \begin{cases} N^{(3\gamma+1)/(\gamma^2-1)} & \text{for } 2 < \gamma < 3 \\ N^{5/(\gamma+1)} & \text{for } 3 < \gamma. \end{cases} \quad (87)$$

With Eqs. (77), (42), (44), and (87) we can finally give the asymptotic behavior of the *Pearson* coefficient  $r_{\max}$  for large maximally assortative networks,

$$r_{\max} \sim \begin{cases} -N^{(-\gamma+2)/(\gamma-1)} & \text{for } 2 < \gamma < \gamma_r \\ N^{-1/(\gamma^2-1)} & \text{for } \gamma_r < \gamma < 3, \end{cases} \quad (88)$$

with the ‘‘threshold’’ value

$$\gamma_r \approx \frac{1}{2} + \sqrt{17/4} \approx 2.56. \quad (89)$$

According to Eq. (88),  $r_{\max}$  vanishes for large networks. Note that the value of  $r_{\max}$  always remains *negative* for  $\gamma < \gamma_r$ . Following the usual definition of assortativity according to the sign of the *Pearson* coefficient, such networks cannot display assortative mixing at all. For this range of  $\gamma$ , the dissortative part in  $K_{nn}$  is so dominant that it overwhelms the assortative part (see also Fig. 5). Although some of the estimates that lead to Eq. (88) are quite rough, we find good agreement with our simulations, see Fig. 6, where  $r_{\max}$  is shown as a function of network size  $N$  for different values of  $\gamma$ . For  $\gamma=2.1$  and  $\gamma=2.3$  the maximal assortativity  $r_{\max}$  is indeed found to be negative,  $\gamma=2.5$  shows slightly positive values,  $\gamma=2.7$  and  $\gamma=2.9$  clearly positive ones.

## V. DISCUSSION

As we have shown above, the correlation profile of scale-free networks exhibits two limiting cases, representing maximally dissortative and assortative mixing. The corresponding *Pearson* coefficients  $r_{\min}$  and  $r_{\max}$  as given by Eqs. (64) and

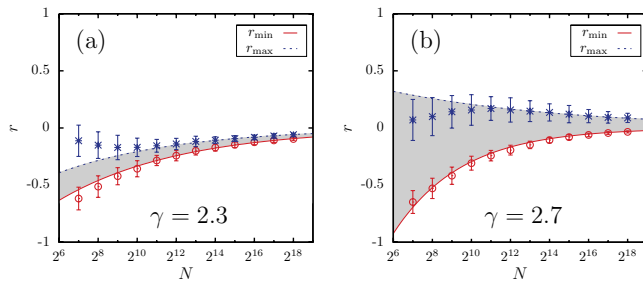


FIG. 7. (Color online) *Pearson* coefficients  $r_{\min}$  and  $r_{\max}$  for maximally correlated networks as a function of network size  $N$  for networks with  $k_0=6$  and scaling exponent (a)  $\gamma=2.3$  and (b)  $\gamma=2.7$ . Data points and fits from relations (64) and (88) are identical to the corresponding curves in Figs. 3 and 6. The shaded areas indicate the range of possible  $r$  values for any realization of a scale-free network with the corresponding parameters  $(N, \gamma, k_0)$ . For networks with  $\gamma=2.3$  as in panel (a), all  $r$  values are negative. In both (a) and (b), the region shrinks to zero for large network size  $N$ .

(88) provide lower and upper bounds for the possible values of  $r$ , as indicated by the shaded area in Fig. 7. The region of possible  $r$  values shrinks with growing network size  $N$ . In the limit of large  $N$ , both  $r_{\min}$  and  $r_{\max}$  vanish, even though the underlying networks are not uncorrelated. Furthermore, it is important to note that networks with  $\gamma \leq \gamma_r$  with  $\gamma_r \approx 2.5$  always exhibit a *negative* correlation coefficient. As discussed in [18,21], this counterintuitive behavior is related to the scaling of  $k_{\max}$  in Eq. (2). The large degree vertices have to export many of their edges into layers of low-degree vertices, giving rise to a dissortative part in the network that eventually dominates the overall structure (see also Fig. 5).

It has been previously recognized that the degree sequence of networks imposes constraints on their correlation

structure and *Pearson* coefficient, see in particular Ref. [28], where such constraints have been illustrated for acyclic and small network graphs. In the present study, we addressed the constraints arising from a scale-free degree sequence and obtained quantitative results for the structure of maximally correlated scale-free networks. Furthermore, we have shown in a quantitative manner how this structure evolves as one varies the network parameters  $N$ ,  $\gamma$ , and  $k_0$ .

We find that these networks are characterized by pronounced communities of vertices with the same or similar degree. Dissortative networks exhibit nested bilayers of vertices with small degree on the one side and vertices with large degree on the other side (see Fig. 1). Counterintuitively, the number of these bilayers does not grow with network size, but saturates for large networks with given parameters  $\gamma$  and  $k_0$  [see Eq. (37)]. In Fig. 4 we also find a layered structure for assortative networks, where layers of low-degree vertices with  $k \leq k_s$  form subgraphs, in which all vertices have the same degree. The number of these monolayers is limited by large degree vertices, which cannot saturate all their edges by connections to vertices with the same degree. This effect decreases with increasing network size and  $k_s$  grows monotonously with  $N$  as in Eq. (75).

In light of these quantitative results on the layered structure of correlated networks, various structural and dynamical phenomena taking place on them may be better understood, since the analysis can possibly be done separately for each layer.

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- [29] For assortative networks, this restriction is essential in order to avoid the trivial case of maximal assortativity, where all vertices are connected only to themselves. In the dissortative case,

multiple connections do not play an important role, since the hubs can saturate all their connections with different low-degree vertices.

- [30] Sometimes the so-called excess degree  $k_{\text{ex}} \equiv k - 1$  is considered instead, which leads to some mathematical simplifications.
- [31] In these cases, one could simply add the few necessary links afterwards if only globally connected networks are desired. Other global properties would hardly be affected by these few links.