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Assortativity of complementary graphs

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Abstract. Newman's measure for (dis)assortativity, the linear degree correlation ρ_D, is widely studied although analytic insight into the assortativity of an arbitrary network remains far from well understood. In this paper, we derive the general relation (2), (3) and Theorem 1 between the assortativity $\rho_D(G)$ of a graph G and the assortativity $\rho_D(G^c)$ of its complement G^c. Both $\rho_D(G)$ and $\rho_D(G^c)$ are linearly related by the degree distribution in G. When the graph $G(N,p)$ possesses a binomial degree distribution as in the Erdős-Rényi random graphs $G_p(N)$, its complementary graph $G_p^c(N) = G_{1-p}(N)$ follows a binomial degree distribution as in the Erdős-Rényi random graphs $G_{1-p}(N)$. We prove that the maximum and minimum assortativity of a class of graphs with a binomial distribution are asymptotically antisymmetric: $\rho_{\max}(N,p) = -\rho_{\min}(N,p)$ for $N \to \infty$. The general relation (3) nicely leads to (a) the relation (10) and (16) between the assortativity range $\rho_{\max}(G) - \rho_{\min}(G)$ of a graph with a given degree distribution and the range $\rho_{\max}(G^c) - \rho_{\min}(G^c)$ of its complementary graph and (b) new bounds (6) and (15) of the assortativity. These results together with our numerical experiments in over 30 real-world complex networks illustrate that the assortativity range $\rho_{\max} - \rho_{\min}$ is generally large in sparse networks, which underlines the importance of assortativity as a network characterizer.

1 Introduction

"Mixing" in complex networks [1,2] refers to the tendency of network nodes to connect preferentially to other nodes with either similar or opposite properties. Networks, where nodes preferentially connect to nodes with (dis)similar property, are called (dis)assortative. When the property of interest is the degree of a node, the linear degree correlation coefficient ρ_D measures the assortativity in node degree of a network, which is computed in [3] as

$$\rho_D = 1 - \frac{\sum_{i\sim j}(d_i - d_j)^2}{\sum_{i=1}^{N} d_i^3 - \frac{1}{2L}\left(\sum_{i=1}^{N} d_i^2\right)^2} \quad (1)$$

where d_j is the degree of node j and $i \sim j$ denotes that node i and j are linked. For example, networks, where high-degree nodes preferentially connect to other high-degree nodes, are assortative ($\rho_D > 0$), whereas networks, where high-degree nodes connect to low-degree nodes, are disassortative ($\rho_D < 0$).

The assortativity was widely studied after it was realized that the degree distribution alone provides an insufficient characterization of complex networks. Networks with the same degree distribution may still differ significantly in various topological features. Consequently, many investigations have focused on (a) exploring the relation between assortativity and other topological properties as well as spectra of networks [3–5] and (b) understanding the effect of assortativity on dynamic network processes such as the epidemic spreading [6] and percolation phenomena [7]. Relations between degree correlation and other topological or dynamic features are mostly studied experimentally [4] or in a specific network model [6,7]. Recently, we have verified spectral bounds for the assortativity [3] and we have studied how the modularity changes under degree-preserving rewiring [8], which alters the assortativity of the graph.

Analytic insight in degree correlations in an arbitrary network is still lacking. In this work, we analytically explore the relation between the assortativity $\rho_D(G)$ of graph G and $\rho_D(G^c)$ of its complement G^c. Let G be a graph or a network and let $\mathcal{N}$ denote the set of $N = |\mathcal{N}|$ nodes and $\mathcal{L}$ the set of $L = |\mathcal{L}|$ links. An undirected graph G can be represented by an $N \times N$ symmetric adjacency matrix A, consisting of elements a_{ij} that are either one or zero depending on whether there is a link between node i and j, or not. The complement G^c of G is a graph containing all the nodes in G and all the links that are *not* in G. Thus, the adjacency matrix of G^c is $A(G^c) = J - I - A(G)$, where J is the all-one matrix and I is the identity matrix.

Furthermore, the general relation (3) between $\rho_D(G)$ and $\rho_D(G^c)$ that we derived is further applied to the complementary classes of graphs with a binomial degree distribution. The binomial degree distribution is a characteristic of an Erdős-Rényi random graph $G_p(N)$, which

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has N nodes and any two nodes are connected independently with a probability p. Such a random construction leads to a zero assortativity as proved in [3]. However, the class of graphs $G(N, p)$ with the same binomial degree distribution $\Pr[D_G = k] = \binom{N-1}{k} p^k (1-p)^{N-1-k}$ as Erdős-Rényi random graphs $G_p(N)$ and obtained, for instance, by degree-preserving rewiring features an assortativity that may vary within a wide range between $\min \rho_D$ and $\max \rho_D$. The complementary class $G(N, 1-p)$ possesses also a binomial degree distribution $\Pr[D_{G^c} = k] = \binom{N-1}{k} (1-p)^k p^{N-1-k}$ characterized by N and $1-p$. We derive the relation between the assortativity of a graph with a binomial degree distribution and that of its complementary graph. This relation enabled us to prove, interestingly, that the maximum and minimum achievable assortativity of a class of graphs with a binomial degree distribution is symmetric around 0, $\max \rho_D(N, p) = -\min \rho_D(N, p)$, which is also numerically illustrated.

The general relation (3) between $\rho_D(G)$ and $\rho_D(G^c)$ also allows us to derive new bounds of the assortativity and to relate the assortativity ranges $\max \rho_D(G) - \min \rho_D(G)$ and $\max \rho_D(G^c) - \min \rho_D(G^c)$ of two complementary classes of graphs, each with a given degree vector or a degree distribution.

The importance of investigating the assortativity and assortativity range relation of complementary graphs lies in the following aspects. (A) Computational complexity of assortative (disassortative) degree-preserving rewiring, which increases (decreases) the assortativity of network whilst the degree of each node remains the same, is higher in a dense network than that in a sparse network [3,9]. Most real-world networks are sparse. However, hierarchical networks at a higher aggregation level tend to be denser. Moreover, most studied brain networks and biological networks are originally weighted networks. These networks are usually transformed into an unweighted network by different link weight thresholds so that classical networking theories can be applied. For each weighted network, unweighted networks usually have to derived at different link densities without loosing the information of the weighted network. Thus, they can be dense with link density ranging over $0.5 < p \ll 1$ and they may even follow a binomial degree distribution [10]. Hence, the assortativity relation between complementary graphs allows the assortative (disassortative) degree-preserving rewiring in a dense network to be derived from the disassortative (assortative) rewiring in its complement with less computational complexity. (B) The maximum $\max \rho_D$ and minimum $\min \rho_D$ assortativity reveals to what extent a degree vector d may characterize a graph. A small range $\max \rho_D - \min \rho_D$ emphasizes the determinant role of the degree vector d, whereas the opposite underlines the importance of the assortativity. Also, experiments suggest that most complex networks (see Tab. E.1 in Appendix E) can be degree-preservingly rewired in two opposite ways so that $\rho_D < 0$ and, alternatively, so that $\rho_D > 0$. Given this experimental observation, we can say that $\max \rho_D > 0$ and $\min \rho_D < 0$ for the degree vector d of a complex network. Consequently, a small $\max \rho_D - \min \rho_D$ means that the degree vector is "hard" to correlate, because ρ_D needs to be close to zero. Apart from degree vectors $d = ru$ of regular graphs of degree r, where u is the all-one vector and $d_j = r$ for each component/node j, it would be interesting to find examples of degree vectors of *complex networks* for which $\min \rho_D > 0$. Such degree vectors would generate and characterize a class of strict assortative graphs, where $\min \rho_D > 0$. A non-trivial example of a strict disassortative class of (almost) regular graphs is analyzed in Appendix D, while Table E.1 in Appendix E shows a couple of real-world complex networks that generate a strict disassortative class. The difference $\max \rho_D - \min \rho_D$ may be regarded as a metric of a given degree vector d that reflects the adaptivity in (dis)assortativity under degree-preserving rewiring. Moreover, the quantity

$$r_G = \frac{\max \rho_D - \rho_D}{\max \rho_D - \min \rho_D}$$

determines the relative maximum assortativity deficiency of a graph, which measures the remaining degree-preserving rewiring left to achieve the maximum assortative state. If degree-preserving rewiring can be considered as an evolutionary process of a network, then r_G quantifies the life-time or the evolutionary state of the network. For example, the functional human brain network of a newly born baby is approximately randomized, with $\rho_D \approx 0$. The learning process rewires the brain and changes ρ_D. Suppose that learning during growth increases ρ_D in that it structures the functional brain, then $1 - r_G$ measures the effect of learning. The maximum possible trained functional brain possesses an assortativity of $\max \rho_D$, which corresponds to learning efficiency $1 - r_G$ equal to 1.

2 Assortativity of complementary graphs

2.1 Related by degree sequence

A node i with degree d_i in graph G has degree $N - 1 - d_i$ in the corresponding complementary graph G^c. All connected node pairs in G^c are non-connected node pairs $i \nsim j$ in G. Therefore, the assortativity of the complementary graph can be written from (1) as

$$\rho_D(G^c) = 1 - \frac{\sum_{i \nsim j} (d_i - d_j)^2}{\sum_{i=1}^{N} (N-1-d_i)^3 - \frac{1}{N(N-1)-2L} \left(\sum_{i=1}^{N} (N-1-d_i)^2 \right)^2}$$

where d_i refers to the degree of node i in the original graph G. The variance $\mathrm{Var}[D] = \sigma^2[D]$ of the degree D of an arbitrary node[1] can be written as a function of the degree differences between all node pairs

$$\sigma^2[D] = \sum_{j=2}^{N} \sum_{k=1}^{j-1} \left(\frac{d_j - d_k}{N} \right)^2$$

[1] We use capital letters for random variables and small letters for specific realizations.

which is derived in [11]. Furthermore, since

$$N^2\sigma^2[D] = N^2\left(E[D^2] - E^2[D]\right) = N\sum_{i=1}^{N} d_i^2 - 4L^2$$

we have

$$\sum_{i\sim j}(d_i - d_j)^2 + \sum_{i\nsim j}(d_i - d_j)^2 = N\sum_{i=1}^{N} d_i^2 - 4L^2.$$

Hence,

$$\rho_D(G^c) = 1 - \rho_D(G) \times \left(\frac{\sum_{i=1}^{N} d_i^3 - \frac{1}{2L}\left(\sum_{i=1}^{N} d_i^2\right)^2}{\sum_{i=1}^{N}(N-1-d_i)^3 - \frac{1}{N(N-1)-2L}\left(\sum_{i=1}^{N}(N-1-d_i)^2\right)^2} \right) + \frac{\left(\sum_{i=1}^{N} d_i^3 - \frac{1}{2L}\left(\sum_{i=1}^{N} d_i^2\right)^2\right) - \left(N\sum_{i=1}^{N} d_i^2 - 4L^2\right)}{\sum_{i=1}^{N}(N-1-d_i)^3 - \frac{1}{N(N-1)-2L}\left(\sum_{i=1}^{N}(N-1-d_i)^2\right)^2} \quad (2)$$

where (1) has been introduced.

2.2 Related by degree distribution

We can rephrase expression (2) in terms of random variables. According to [3],

$$\sum_{i=1}^{N} d_i^3 - \frac{1}{2L}\left(\sum_{i=1}^{N} d_i^2\right)^2 = 2L\sigma^2\left[D_{l^+}(G)\right]$$

$$\sum_{i=1}^{N}(N-1-d_i)^3 - \frac{1}{N(N-1)-2L} \times \left(\sum_{i=1}^{N}(N-1-d_i)^2\right)^2 = \left(N(N-1)-2L\right)\sigma^2\left[D_{l^+}(G^c)\right]$$

$$N\sum_{i=1}^{N} d_i^2 - 4L^2 = N^2\sigma^2[D]$$

where $\sigma^2[D_{l^+}(G)]$ and $\sigma^2[D_{l^+}(G^c)]$ are the variances of the degrees at one side of an arbitrary link in G and in G^c, respectively. Thus, (2) becomes

$$\rho_D(G^c) = -\rho_D(G)\frac{2L\sigma^2\left[D_{l^+}(G)\right]}{\left(N(N-1)-2L\right)\sigma^2\left[D_{l^+}(G^c)\right]} + 1 - \frac{N^2\sigma^2[D(G)] - 2L\sigma^2\left[D_{l^+}(G)\right]}{\left(N(N-1)-2L\right)\sigma^2\left[D_{l^+}(G^c)\right]} \quad (3)$$

which holds for any graph. Observe that, except for $\rho_D(G)$, all factors and terms in (2) and (3) are constant for a given degree vector. This means that the assortativity $\rho_D(G^c)$ of the complement G^c of a graph linearly varies with the assortativity $\rho_D(G)$ of the graph G, and vice versa.

Theorem 1. *The assortativity relation between complementary graphs (3) can be further expressed as a function of the degree distribution* $\Pr[D=k]$ *in the original graph* G *where*

$$\frac{2L\sigma^2\left[D_{l^+}(G)\right]}{\left(N(N-1)-2L\right)\sigma^2\left[D_{l^+}(G^c)\right]} = \frac{E[D^3] - \frac{E^2[D^2]}{E[D]}}{\frac{(N-1)^2E[D^2]-(N-1)^2E^2[D]+(N-1)E[D^2]E[D]-E^2[D^2]}{(N-1-E[D])} - E[D^3]} \quad (4)$$

$$\frac{N^2\sigma^2[D(G)] - 2L\sigma^2\left[D_{l^+}(G)\right]}{\left(N(N-1)-2L\right)\sigma^2\left[D_{l^+}(G^c)\right]} = \frac{NE[D^2] - NE^2[D] - E[D^3] + \frac{E^2[D^2]}{E[D]}}{\frac{(N-1)^2E[D^2]-(N-1)^2E^2[D]+(N-1)E[D^2]E[D]-E^2[D^2]}{(N-1-E[D])} - E[D^3]}. \quad (5)$$

Proof. See Appendix A. □

Relations (2), (3) and Theorem 1 are equivalent and explicitly reflect how the assortativity $\rho_D(G^c)$ and $\rho_D(G)$ of complementary graphs are linearly related.

2.3 Bounds for the assortativity

Given a degree distribution or degree sequence, the assortativity $\rho_D(G)$ of a graph may range within

$$-1 \le \min\rho_D \le \rho_D(G) \le \max\rho_D \le 1$$

and, likewise, the assortativity of its complementary graph $\rho_D(G^c)$ may vary within

$$-1 \le \min\rho_D^c \le \rho_D(G^c) \le \max\rho_D^c \le 1$$

where $\max\rho_D$ and $\min\rho_D$ ($\max\rho_D^c$ and $\min\rho_D^c$) are the maximum and minimum achievable assortativity of the (complementary) class of graphs with a given degree vector d.

When $\rho_D(G) = -1$, (3) shows, that

$$4L\sigma^2\left[D_{l^+}(G)\right] \le N^2\sigma^2[D(G)] \le 2N(N-1)\sigma^2\left[D_{l^+}(G^c)\right]$$

and, when $\rho_D(G) = 1$, that

$$N^2\sigma^2[D(G)] \le 2\left(N(N-1)-2L\right)\sigma^2\left[D_{l^+}(G^c)\right].$$

Thus, if $\min\rho_D = -1$ and $\max\rho_D = 1$,

$$4L\sigma^2\left[D_{l^+}(G)\right] \le N^2\sigma^2[D(G)] \le 2\left(N(N-1)-2L\right)\sigma^2\left[D_{l^+}(G^c)\right].$$

Alternatively, after inverting (3),

$$\rho_D(G) = -\frac{(N(N-1)-2L)\,\sigma^2\left[D_{l+}(G^c)\right]}{2L\sigma^2\left[D_{l+}(G)\right]}\rho_D(G^c) + 1 - \frac{N^2\sigma^2\left[D(G)\right] - (N(N-1)-2L)\,\sigma^2\left[D_{l+}(G^c)\right]}{2L\sigma^2\left[D_{l+}(G)\right]}$$

we find the bounds for the assortativity and disassortativity of any graph G,

$$\mathfrak{r}_{\min} \leq \rho_D(G) \leq \mathfrak{r}_{\min} + \frac{(N(N-1)-2L)\,\sigma^2\left[D_{l+}(G^c)\right]}{L\sigma^2\left[D_{l+}(G)\right]} \tag{6}$$

where

$$\mathfrak{r}_{\min} = 1 - \frac{N^2\sigma^2\left[D(G)\right]}{2L\sigma^2\left[D_{l+}(G)\right]} = 1 - \frac{N\sigma^2\left[D(G)\right]}{p(N-1)\sigma^2\left[D_{l+}(G)\right]} \approx 1 - \frac{1}{p}\frac{\sigma^2\left[D(G)\right]}{\sigma^2\left[D_{l+}(G)\right]}. \tag{7}$$

Thus, we conclude that

$$\min \rho_D \geq \max\left(-1, \mathfrak{r}_{\min}\right) \tag{8}$$

$$\max \rho_D \leq \min\left(1, \mathfrak{r}_{\min} + \frac{2\,(1-p)}{p}\frac{\sigma^2\left[D_{l+}(G^c)\right]}{\sigma^2\left[D_{l+}(G)\right]}\right)$$

where $p = L/\binom{N}{2}$ is the link density. The assortativity range $0 \leq \max\rho_D - \min\rho_D \leq 2$ of the class of graphs G and the assortativity range $0 \leq \max\rho_D^c - \min\rho_D^c \leq 2$ of its complementary class can be related by (3) as

$$(\max\rho_D^c - \min\rho_D^c) = \frac{2L\sigma^2\left[D_{l+}(G)\right]}{(N(N-1)-2L)\,\sigma^2\left[D_{l+}(G^c)\right]} \times (\max\rho_D - \min\rho_D) \tag{9}$$

or, inverted

$$(\max\rho_D - \min\rho_D) = \left(\frac{1}{p} - 1\right)\frac{\sigma^2\left[D_{l+}(G^c)\right]}{\sigma^2\left[D_{l+}(G)\right]} \times (\max\rho_D^c - \min\rho_D^c) \tag{10}$$

where both $\sigma^2\left[D_{l+}(G^c)\right]$ and $\sigma^2\left[D_{l+}(G)\right]$ have been expressed as a function of the degree distribution of the original graph in Appendix A. The assortativity range $\max\rho_D - \min\rho_D$ is small if (a) the variance $\sigma^2\left[D_{l+}(G^c)\right]$ is small, (b) $\sigma^2\left[D_{l+}(G)\right]$ is large and/or the link density p is high (close to 1).

The ratio $\frac{\sigma^2\left[D_{l+}(G^c)\right]}{\sigma^2\left[D_{l+}(G)\right]}$ has been extensively analyzed in Appendix A, in general as well as in graphs with a binomial or a power-law degree distribution. When a graph has a binomial degree distribution $\Pr[D_G = k] = \binom{N-1}{k}p^k(1-p)^{N-1-k}$, $\frac{\sigma^2\left[D_{l+}(G^c)\right]}{\sigma^2\left[D_{l+}(G)\right]} = 1$ as derived both in Section 3.1 (rigorously) and in Appendix B (asymptotically). When a graph has a power-law degree distribution $\Pr[D = k] = ck^{-\alpha}$, where $c = 1/\sum_{k=1}^{N-1}k^{-\alpha}$ and $1 \leq \alpha \leq 3$, $\frac{\sigma^2\left[D_{l+}(G^c)\right]}{\sigma^2\left[D_{l+}(G)\right]} \to 0$ if the graph is large and sparse

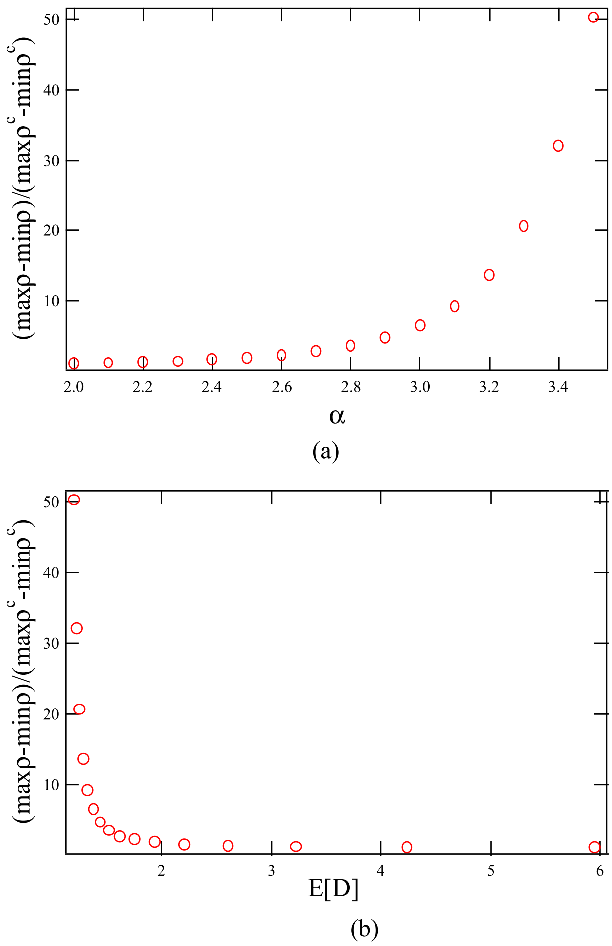

Fig. 1. (Color online) The ratio $\Delta = \frac{\max\rho_D - \min\rho_D}{\max\rho_D^c - \min\rho_D^c}$ in graphs with $N = 10\,000$ nodes and with a power-law degree distribution versus (a) the exponent α of the degree distribution and versus (b) the average degree $E[D]$.

as proved in Appendix B. We further quantitatively investigate the assortativity range ratio

$$\Delta = \frac{\max\rho_D - \min\rho_D}{\max\rho_D^c - \min\rho_D^c} = \left(\frac{1}{p} - 1\right)\frac{\sigma^2\left[D_{l+}(G^c)\right]}{\sigma^2\left[D_{l+}(G)\right]}$$

in graphs with a power-law or binomial degree distribution. In binomial graphs, $\Delta = \frac{1}{p} - 1$. In graphs with $N = 10\,000$ nodes and with a power-law degree distribution, the ratio Δ, expressed as a function of the degree distribution, can be numerically computed. We consider power-law graphs with an exponent $2 \leq \alpha \leq 3.5$, since most real-world graphs have $2 \leq \alpha \leq 3$. As shown in Figure 1a, the ratio of the assortativity range Δ increases as the power exponent α, or the heterogeneity increases. The assortativity of the compliment may still vary within a certain range upbounded by $2/\Delta$ when $2 \leq \alpha \leq 3$, whereas $2/\Delta$ goes fast to zero when $\alpha > 3$. The link density is smaller for a larger exponent α. Hence, the ratio Δ decreases as the average degree/link density increases, as depicted in Figure 1b.

In general, a sparse network, favors a large assortativity range. This effect of a (small) link density is more evident in graphs with a binomial degree distribution than that in power-law graphs, since $\frac{\sigma^2[D_{l^+}(G^c)]}{\sigma^2[D_{l^+}(G)]}$ is far smaller in power-law graphs. As shown in Figure 3 and 4, a power-law graph, indeed, has a smaller assortativity range compare to the binomial graph with the same link density.

When p is large, a non-trivial bound can be derived from (10)

$$\max\rho_D - \min\rho_D \leq 2\left(\frac{1}{p}-1\right)\frac{\sigma^2[D_{l^+}(G^c)]}{\sigma^2[D_{l^+}(G)]}. \tag{11}$$

Most real-world networks are sparse. However, hierarchical network at a higher aggregation level or the unweighted networks transformed from the original weighted e.g. brain and biological networks, likely have a link density $0.5 < p \ll 1$, as discussed in Section 1. The assortativity of such a dense network can be derived from its complement with less computational complexity by the assortativity relation (2), (3) or Theorem 1. A non-trivial bound of the assortativity range tends to be achieved via the assortativity range relation (10). When $p \to 1$, the range of variability in the degrees of a graph with a number of links $L \sim O(N^2)$ is narrow and the assortativity is close to zero as illustrated in Figure 6.

3 Graphs with a binomial degree distribution

Consider the class of graphs $G(N,p)$ with a binomial degree distribution $\Pr[D_G = k] = \binom{N-1}{k}p^k(1-p)^{N-1-k}$ characterized by N and p as in the Erdős-Rényi (ER) random graphs $G_p(N)$. Its complementary class of graphs $G(N,1-p)$ also possess a binomial degree distribution $\Pr[D_{G^c} = k] = \binom{N-1}{k}(1-p)^k p^{N-1-k}$ with parameter N and $1-p$ as followed by the ER random graphs $G_{1-p}(N)$. The assortativity of connected ER random graphs is zero [3]. However, the assortativity of graphs like $G(N,p)$ conditioned only by a degree distribution can vary with in a large range. Besides its theoretical beauty, the binomial distribution has been observed in e.g. peer-to-peer networks [12] and the unweighted functional brain networks [10].

3.1 Assortativity of complementary graphs

We first explore the relation between the assortativity $\rho_D(G(N,p))$ and $\rho_D(G^c(N,p)) = \rho_D(G(N,1-p))$ of two complementary graphs each having a binomial degree distribution characterized by (N,p) and $(N,1-p)$ respectively, based on Theorem 1.

For a binomial degree distribution $\Pr[D_G = k] = \binom{N-1}{k}p^k(1-p)^{N-1-k}$, it follows that

$$E[D^3] = (N-1)p(1-6p+3Np+6p^2-5Np^2+N^2p^2)$$
$$E[D^2] = (N-1)p(1-2p+Np)$$
$$E[D] = (N-1)p.$$

Substituted into Theorem 1 and further into (3), we find

$$\frac{\sigma^2[D_{l^+}(G^c)]}{\sigma^2[D_{l^+}(G)]} = 1 \tag{12}$$

$$\begin{aligned}\rho_D(G^c(N,p)) &= \rho_D(G(N,1-p)) \\ &= -\frac{p}{1-p}\rho_D(G(N,p)) - \frac{2}{(N-2)(1-p)}.\end{aligned} \tag{13}$$

If a graph with a binomial degree distribution is assortative $\rho_D(G(N,p)) > 0$, its complementary graph is definitely disassortative $\rho_D(G^c(N,p)) < 0$, because $\frac{2}{(N-2)(1-p)} > 0$. The reverse does not hold when N is small. However, the bound

$$\rho_D(G(N,1-p)) \leq -\frac{p}{1-p}\rho_D(G(N,p))$$

is attained asymptotically for $N \to \infty$,

$$\lim_{N\to\infty}\rho_D(G(N,1-p)) = -\frac{p}{1-p}\lim_{N\to\infty}\rho_D(G(N,p)). \tag{14}$$

Moreover, from (14), we obtain the bounds

$$\max\left(-1, 1-\frac{1}{p}\right) \leq \lim_{N\to\infty}\rho_D(G(N,p)) \leq \min\left(1, \frac{1}{p}-1\right) \tag{15}$$

demonstrating that $\lim_{N\to\infty,p\to 1}\rho_D(G(N,p)) = 0$. In other words, the linear degree correlation coefficient of the complete graph is zero. Only for $p > \frac{1}{2}$, these bounds (15) are non-trivial. When p is small, a large assortativity range can be expected.

3.2 Maximum and minimum assortativity

Given a class of graphs with a binomial degree distribution $\Pr[D_G = k] = \binom{N-1}{k}p^k(1-p)^{N-1-k}$, the maximal and minimal achievable assortativity is denoted by $\max\rho(N,p)$ and $\min\rho(N,p)$. The complementary class of graphs achieve the maximal and minimal assortativity $\max\rho(N,1-p)$ and $\min\rho(N,1-p)$. Relation (13) shows that $\max\rho(N,1-p) = -\frac{p}{1-p}\min\rho(N,p)$ and $\min\rho(N,1-p) = -\frac{p}{1-p}\max\rho(N,p)$. Thus,

$$\begin{aligned}\max\rho(N,1-p) - \min\rho(N,1-p) = \frac{p}{1-p}&(\max\rho(N,p) \\ &- \min\rho(N,p))\end{aligned} \tag{16}$$

which is a special case of (9) for graphs with a binomial degree distribution. When p is small, the assortativity range is far larger than that in the complementary class of graphs. The complementary classes of graphs $G(N,p)$ and $G(N,1-p)$ both follow a binomial degree distribution. They differ only in link density p. A small link density p contributes to a wide range of assortativity as illustrated in Figure 2.

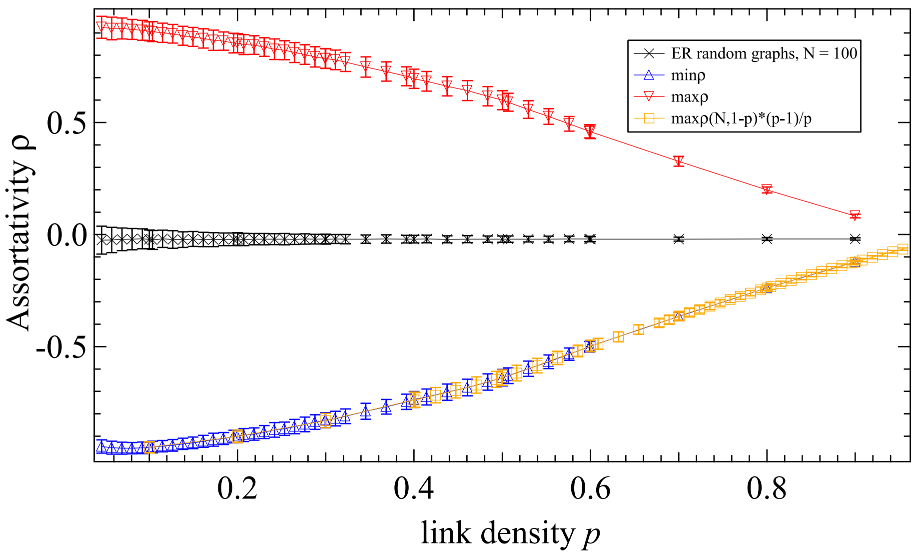

Fig. 2. (Color online) The average maximum $\max\rho(N=100,p)$ and minimum $\min\rho(N=100,p)$ assortativity of graphs with a binomial degree distribution versus the link density p. Verification of (14): $\frac{p-1}{p}\max\rho(N,p) = \min\rho(N,p)$.

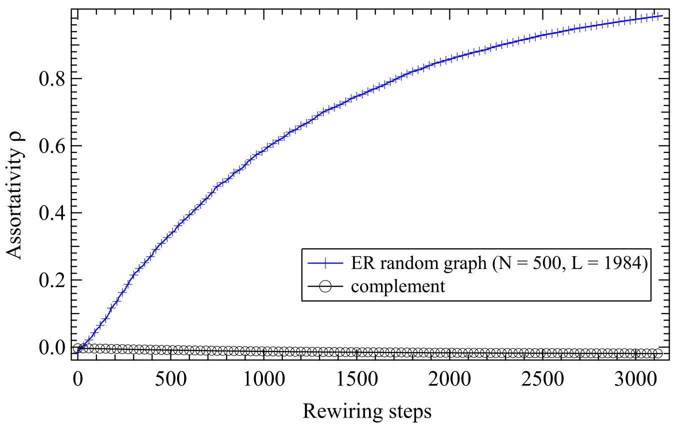

Fig. 3. (Color online) The assortativity of the Erdős-Rényi random graph with $N = 500$ nodes and $L = 1984$ links and its complement versus the number of rewiring steps in an assortative degree-preserving rewiring procedure.

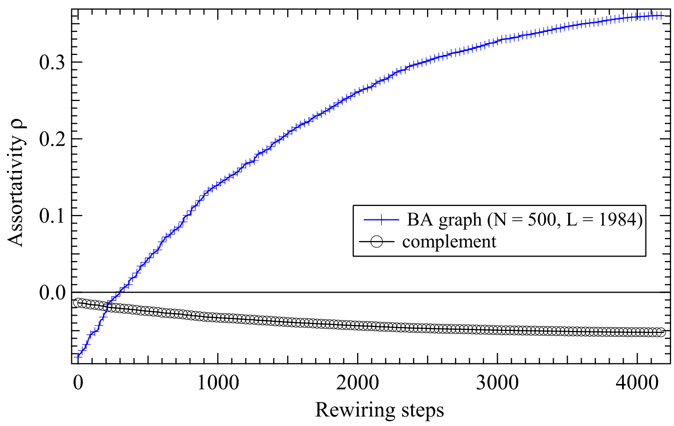

Fig. 4. (Color online) The assortativity of the Barabási-Albert random graph with $N = 500$ nodes and $L = 1984$ links and its complement versus the number of rewiring steps in an assortative degree-preserving rewiring procedure.

Most real-world networks are mostly sparse. Thus, their assortativity ranges expected to be larger than that of their corresponding complementary graphs according to (10) and (16). Furthermore, we will prove the following theorem:

Theorem 2. *For binomially distributed nodal degrees, the maximum* $\rho_{\max}(N,p)$ *and minimum assortativity* $\rho_{\min}(N,p)$ *tend to be symmetric around the* $\rho_D = 0$ *axis for large* N*. Specifically, it holds that*

$$\lim_{N\to\infty} \max\rho(N,p) + \min\rho(N,p) = 0$$

when the link density $p \in (0,1)$.

Proof. See Appendix C. □

Numerical computations in Figure 2, indeed, illustrate that, approximately for finite N,

$$\max\rho(N,p) \simeq -\min\rho(N,p)$$

for any link density p. The values of $\max\rho(N,p)$ and $\min\rho(N,p)$ in Figure 2 are computed with the exact algorithm explained in [3].

4 Real-world complex networks

This section illustrates how the assortativity of a graph and of its complement changes under degree-preserving rewiring, during which the degree of each node in the graph does not change. Figure 3 shows that, for an ER random graph with $N = 500$ nodes, $L = 1984$ links and link density $p = 0.016$, the assortativity of the complement decreases much slower than that the assortativity of the original graph increases under degree-preserving rewiring. Relation (3), indeed, confirms that the assortativity of the complement must decrease, when $\rho_D(G)$ increases. The slower observed speed is due to the factor $\frac{p}{1-p}$ in (13) which is small for a small p. In general, assortativity of

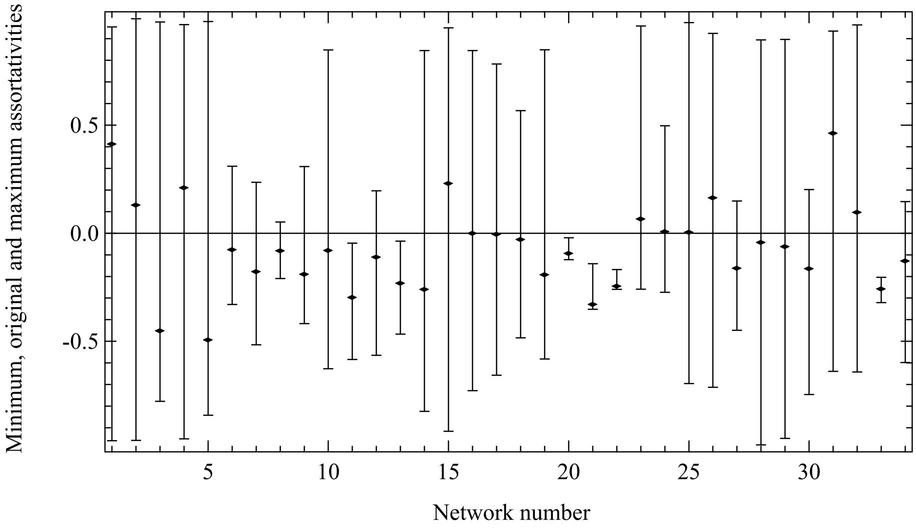

Fig. 5. The minimum ($\min \rho$), original (ρ_D) and maximum ($\max \rho$) assortativity for various complex networks, described in Appendix E. The values are computed by a heuristic, greedy degree-preserving rewiring algorithm.

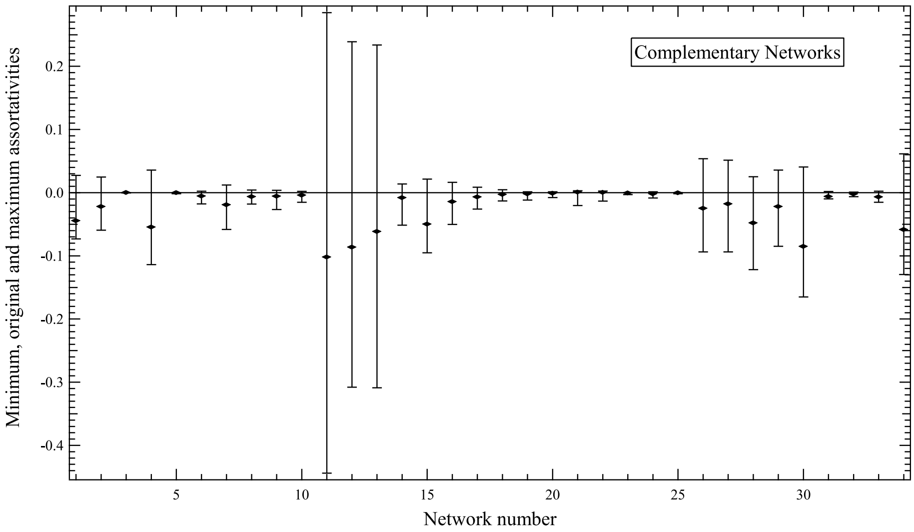

Fig. 6. The minimum ($\min \rho$), original (ρ_D) and maximum ($\max \rho$) assortativity for the complements of various complex networks, described in Appendix E. The values are derived from those of Figure 5 by (2). They can be equivalently computed by the heuristic, greedy degree-preserving rewiring algorithm.

the complement changes much slower than that the assortativity of the original graph changes under degree-preserving rewiring, if the factor $\frac{2L\sigma^2\left[D_{l+}(G)\right]}{(N(N-1)-2L)\sigma^2\left[D_{l+}(G^c)\right]}$ in relation (3), which is a constant under degree-preserving rewiring, is small.

The relation (16) and Figure 2 demonstrate that a small link density (as in Fig. 3) corresponds to a large assortativity range $\max \rho - \min \rho$ and that the corresponding link density $1 - p$ in the complement leads to a small $\rho_{\max} - \rho_{\min}$. This also explains in Figure 3 why the assortativity of the graph increases much faster than the corresponding decrease in the complement during the degree-preserved rewiring process. Figure 4 shows the same tendency in a Barabási-Albert graph [13] of the same size (N and L).

Figure 5 illustrates for over thirty real-world complex networks how the assortativity ρ_D lies within the maximum possible range $\rho_{\max} - \rho_{\min}$. As shown in the corresponding Table E.1, the link density $p = L/\binom{N}{2} = \frac{E[D]}{N-1}$ in these complex networks is small, ranging from $4 \times 10^{-4} \leq p \leq 0.37$, such that the bound (11) for the assortativity range $\max \rho - \min \rho$ is here not confined by p. We observe that there are 6 strict disassortative networks, where $\rho_{\max} < 0$. The assortativity range in those networks is small compared to the majority of complex networks. Moreover, they seem to possess a few very large degree nodes and many small degree nodes. So far, we have not found a strict assortative network, where $\min \rho > 0$. This observation supports the explanation in [3] why most real-world networks favor disassortativity due to a stronger connectivity and higher diversity than in assortative graphs. It would be interesting to know whether strict assortative, connected complex networks actually do exist. Assortativity range of the complements of these real-world networks, as shown in Figure 6, are mostly small and around zero. This is due to the effect of a large link density p on the assortativity range relation between complementary graphs (10). However, the degree distribution plays an important role in determining the

$$E[D_{l^+}(G^c)] = \sum_{k=0}^{N-1} \frac{k^2 \Pr[D = N-1-k]}{N-1-E[D]} = \frac{(N-1)^2 + E[D^2] - 2(N-1)E[D]}{N-1-E[D]}$$

$$E[D^2_{l^+}(G^c)] = \frac{(N-1)^3 + 3(N-1)E[D^2] - 3(N-1)^2 E[D] - E[D^3]}{N-1-E[D]}$$

$$\sigma^2\left[D_{l^+}(G^c)\right] = \frac{(N-1)^2 E[D^2] - (N-1)E[D^3] + (N-1)E[D^2]E[D] - (N-1)^2 E^2[D] + E[D^3]E[D] - E^2[D^2]}{(N-1-E[D])^2}.$$

assortativity range, which explains possible large assortativity range even in dense networks (e.g. network 11–13).

5 Conclusion

The general relations (2), (3) and Theorem 1 between the assortativity $\rho_D(G)$ and $\rho_D(G^c)$ of two complementary graphs are considered important new findings. Based on these relations, we further derive, bounds for the assortativity (6) and the relation (9) between assortativity range of two complementary graphs with a given degree distribution. The influence of link density and degree distribution on the assortativity and on the assortativity range of two complementary graphs is explicitly revealed.

Properties of complementary graphs are widely studied in Erdős-Rényi (ER) random graphs, because the complementary graph of an ER random graphs $G_p(N)$ is again an Erdős-Rényi random graphs $G_{1-p}(N)$. Actually, the assortativity of an ER random graph is proved in [3] to be zero due to the random construction. However, constrained only by a binomial degree distribution as in the ER random graphs $G_p(N)$, the assortativity of a graph $G(N,p)$ may vary within a wide range. The complementary graph $G(N, 1-p)$ also possesses a binomial degree distribution, but characterized by N and link density $1-p$. The relation between $\rho_D(G(N,p))$ and $\rho_D(G(N,1-p))$ in this case can be simplified into (14). As a consequence, the maximum and minimum assortativity of a class of graphs with a binomial distribution are proved to be symmetric, $\max \rho(N,p) = -\min \rho(N,p)$ and the range $\max \rho(N,p) - \min \rho(N,p)$ is shown in (16) to be smaller for a large p.

A degree distribution is normally considered as a first order metric to characterize a network, while the assortativity as a second order descriptor. A narrow assortativity range $\max \rho - \min \rho$ of graphs with a given degree distribution implies that the degree distribution alone specifies the other properties well and is thus representative. Our results, (10) and (16), illustrate that a high link density confines the possible assortativity range more than a low link density. This, again, strengthens the importance of assortativity as a network characterizer, since most real-world networks are sparse. Finally, in over 30 real-world complex networks, the assortativity range $\max \rho - \min \rho$ is generally found to be large, except for a few strict disassortative graphs ($\max \rho < 0$). As we did not encounter strict assortative graphs ($\min \rho > 0$), it may be worthwhile to ponder whether they exist. Assortativity range relation 10 allows us to derive a non-trivial bound in one of the two complementary graphs, mostly the dense one. Exploring a better assortativity bound for sparse networks is deemed as an interesting future work. The ratio $\frac{\sigma^2\left[D_{l^+}(G^c)\right]}{\sigma^2\left[D_{l^+}(G)\right]}$ in the assortativity range relation has been explicitly expressed as functions of degree moments. Further quantitative studies on this ratio in network models as well as in real-world networks will provides more insights.

Appendix A: Proof of Theorem 1

Consider an arbitrary link l in G with right endnode l^+. The probability that this link l is connected to a node $j = l^+$ with degree k equals

$$\Pr[D_{l^+}(G) = k] = \sum_{j=1}^{N} \Pr\left[\text{node } j \text{ is } l^+ | D_j = k\right] \Pr\left[D_j = k\right].$$

Each link l consists of two half links connected to node l^- and node l^+. With the basic law of the degree is $\sum_{j=1}^{N} D_j = 2L$, we have

$$\Pr\left[\text{node } j \text{ is } l^+ | D_j = k\right] = \frac{k}{2L}.$$

Since each nodal degree D_j is distributed as the degree D of an arbitrary node in G, $\Pr[D_j = k] = \Pr[D = k]$ and we end up with

$$\Pr[D_{l^+}(G) = k] = \frac{Nk \Pr[D = k]}{2L} = \frac{k \Pr[D = k]}{E[D]}$$

$$\Pr[D_{l^+}(G^c) = k] = \frac{k \Pr[D = N-1-k]}{N-1-E[D]}.$$

These expressions allow us to derive $\sigma^2\left[D_{l^+}(G)\right]$ and $\sigma^2\left[D_{l^+}(G^c)\right]$ in (3) as a function of the degree distribution $\Pr[D = k]$:

$$E[D_{l^+}(G)] = \sum_{k=0}^{N-1} \frac{Nk^2 \Pr[D = k]}{2L} = \frac{E[D^2]}{E[D]}$$

$$E[D^2_{l^+}(G)] = \sum_{k=0}^{N-1} \frac{Nk^3 \Pr[D = k]}{2L} = \frac{E[D^3]}{E[D]}$$

$$\sigma^2\left[D_{l^+}(G)\right] = \frac{E[D^3]E[D] - E^2[D^2]}{E^2[D]}.$$

Similarly,

See equation above.

They, together, lead to Theorem 1.

$$\frac{\mu_3}{\mu_2} = \frac{\sum_{k=1}^{N-1} k^{-(\alpha-3)} - 3c\sum_{k=1}^{N-1} k^{-(\alpha-1)} \sum_{k=1}^{N-1} k^{-(\alpha-2)} - c^2\left(\sum_{k=1}^{N-1} k^{-(\alpha-1)}\right)^3}{\sum_{k=1}^{N-1} k^{-(\alpha-2)} - c\left(\sum_{k=1}^{N-1} k^{-(\alpha-1)}\right)^2}$$

$$\simeq \frac{\frac{1-N^{4-\alpha}}{\alpha-4} - 3\frac{\alpha-1}{1-N^{1-\alpha}}\frac{1-N^{2-\alpha}}{\alpha-2}\frac{1-N^{3-\alpha}}{\alpha-3} - \left(\frac{\alpha-1}{1-N^{1-\alpha}}\right)^2\left(\frac{1-N^{2-\alpha}}{\alpha-2}\right)^3}{\frac{1-N^{3-\alpha}}{\alpha-3} - \frac{\alpha-1}{1-N^{1-\alpha}}\left(\frac{1-N^{2-\alpha}}{\alpha-2}\right)^2}.$$

Appendix B: The ratio $\frac{\sigma^2[D_{l^+}(G^c)]}{\sigma^2[D_{l^+}(G)]}$

The ratio $\frac{\sigma^2[D_{l^+}(G^c)]}{\sigma^2[D_{l^+}(G)]}$ can be written as a function of the moments of the degree is the original graph G

$$\frac{\sigma^2[D_{l^+}(G^c)]}{\sigma^2[D_{l^+}(G)]} = \frac{E^2[D]}{(N-1-E[D])^2} + (N-1) \times \frac{(N-1)\mathrm{Var}[D] - \{E[D^3]-E[D^2]E[D]\}}{(N-1-E[D])^2} \times \frac{E^2[D]}{E[D^3]E[D]-E^2[D^2]}.$$

We express the variances $\sigma^2[D_{l^+}(G^c)]$ and $\sigma^2[D_{l^+}(G)]$ in terms of the centered moments $\mu_k = E[(D-E[D])^k]$ for $k \geq 2$. In particular, denoting the average degree by $\mu = E[D]$, we have that

$$\begin{aligned} E[D^2] &= \mu_2 + \mu^2 = \mu^2 + \mathrm{Var}[D] \\ E[D^3] &= E[(D-\mu+\mu)^3] \\ &= E[(D-\mu)^3 + 3(D-\mu)^2\mu + 3(D-\mu)\mu^2 + \mu^3] \\ &= \mu_3 + \mu^3 + 3\mu_2\mu = \mu^3 + 3\mu\mathrm{Var}[D] + \mu_3 \end{aligned}$$

where the skewness $\frac{\mu_3}{\mu_2^{3/2}}$ measures the lack of symmetry of the degree distribution around the mean. Then,

$$\begin{aligned} \frac{\sigma^2[D_{l^+}(G^c)]}{\sigma^2[D_{l^+}(G)]} &= \frac{\mu^2}{(N-1-\mu)^2} + (N-1) \times \frac{(N-1)\mu_2 - \{\mu_3 + \mu^3 + 2\mu_2\mu\}}{(N-1-\mu)^2} \times \frac{\mu^2}{\mu_3\mu + \mu_2\mu^2 - \mu_2^2} \\ &= \frac{\mu^2}{(N-1-\mu)^2} + (N-1) \times \frac{(N-1-2\mu)\mu_2 - \mu_3 - \mu^3}{(N-1-\mu)^2} \times \frac{1}{\frac{\mu_3}{\mu} + \mu_2\left(1-\frac{\mu_2}{\mu^2}\right)} \\ &= \frac{\mu^2}{(N-1-\mu)^2} + \frac{\mu_2 - \frac{\mu_3+\mu^3}{N-1-2\mu}}{\frac{(N-1-\mu)^2}{(N-1)(N-1-2\mu)}\left(\left(1-\frac{\mu_2}{\mu^2}\right)\mu_2 + \frac{\mu_3}{\mu}\right)}. \end{aligned}$$

We consider large and sparse graphs such that

$$\frac{\sigma^2[D_{l^+}(G^c)]}{\sigma^2[D_{l^+}(G)]} = \frac{1-\frac{\mu_3+\mu^3}{N\mu_2}}{\left(1-\frac{\mu_2}{\mu^2}\right)+\frac{\mu_3}{\mu\mu_2}}. \tag{B.1}$$

When the degree distribution is symmetrical around the mean such that $\mu_3 = 0$,

$$\frac{\sigma^2[D_{l^+}(G^c)]}{\sigma^2[D_{l^+}(G)]} = \frac{\mu^2}{\mu^2-\mu_2}.$$

Moreover, if the symmetrical degree distribution follows a binomial distribution where $\mu = Np$ and $\mu_2 = \mu(1-p)$,

$$\frac{\sigma^2[D_{l^+}(G^c)]}{\sigma^2[D_{l^+}(G)]} = 1$$

which is the same as (12), rigorously derived in Section 3.1.

For a power-law distribution $\Pr[D=k] = ck^{-\alpha}$ and $c = \frac{1}{\sum_{k=1}^{N-1} k^{-\alpha}} \simeq \frac{1}{\zeta(\alpha)}$, we have that $E[D] = \mu = c\sum_{k=1}^{N-1} k^{-(\alpha-1)} \simeq \frac{\zeta(\alpha-1)}{\zeta(\alpha)}$ and $E[D^m] = c\sum_{k=1}^{N-1} k^{-(\alpha-m)} \simeq \frac{\zeta(\alpha-m)}{\zeta(\alpha)}$, where the approximation sign is only valid provided $\alpha - m > 1$. Then,

$$\begin{aligned} \mu_3 &= E\left[(D-\mu)^3\right] = E\left[D^3\right] - 3\mu E\left[D^2\right] - \mu^3 \\ &= c\sum_{k=1}^{N-1} k^{-(\alpha-3)} - 3c^2\sum_{k=1}^{N-1} k^{-(\alpha-1)} \\ &\quad \times \sum_{k=1}^{N-1} k^{-(\alpha-2)} - c^3\left(\sum_{k=1}^{N-1} k^{-(\alpha-1)}\right)^3. \end{aligned}$$

For large, but finite N, we approximate as

$$\sum_{k=1}^{N-1} k^{-\alpha} \simeq \int_1^N \frac{dx}{x^\alpha} = \frac{N^{1-\alpha}-1}{1-\alpha} = \frac{1-N^{1-\alpha}}{\alpha-1}$$

and

See equation above.

For $1 < \alpha < 2$ and large, but finite N, we have

$$\frac{\mu_3}{\mu_2} \simeq \frac{\frac{N^{4-\alpha}}{4-\alpha} - 3\frac{(\alpha-1)}{(2-\alpha)(3-\alpha)}N^{5-2\alpha} - \frac{(\alpha-1)^2}{(2-\alpha)^3}N^{6-3\alpha}}{\frac{N^{3-\alpha}}{3-\alpha} - \frac{(\alpha-1)}{(2-\alpha)^2}N^{4-2\alpha}}$$

$$= N\frac{\frac{1}{4-\alpha} - 3\frac{(\alpha-1)}{(2-\alpha)(3-\alpha)}N^{1-\alpha} - \frac{(\alpha-1)^2}{(2-\alpha)^3}N^{2(1-\alpha)}}{\frac{1}{3-\alpha} - \frac{(\alpha-1)}{(2-\alpha)^2}N^{1-\alpha}}$$

$$\simeq \frac{3-\alpha}{4-\alpha}N > 0.$$

Similarly,

$$\frac{\mu_3 + \mu^3}{N\mu_2} \simeq \frac{3-\alpha}{4-\alpha}$$

$$\frac{\mu_3}{\mu\mu_2} \simeq \frac{(3-\alpha)(2-\alpha)}{(4-\alpha)(\alpha-1)}N^{\alpha-1}$$

and

$$\frac{\mu_2}{\mu^2} \simeq \frac{\frac{1-\alpha}{\alpha-3}N^{\alpha-1} - \left(\frac{\alpha-1}{\alpha-2}\right)^2}{\left(\frac{\alpha-1}{\alpha-2}\right)^2}.$$

Together with (B.1), we have

$$\frac{\sigma^2\left[D_{l^+}(G^c)\right]}{\sigma^2\left[D_{l^+}(G)\right]} \simeq$$

$$\frac{1-\frac{3-\alpha}{4-\alpha}}{\left(1-\frac{\frac{1-\alpha}{\alpha-3}N^{\alpha-1}-\left(\frac{\alpha-1}{\alpha-2}\right)^2}{\left(\frac{\alpha-1}{\alpha-2}\right)^2}\right)+\frac{(3-\alpha)(2-\alpha)}{(4-\alpha)(\alpha-1)}N^{\alpha-1}}$$

$$= O\left(N^{1-\alpha}\right) \to 0.$$

When $2 < \alpha < 3$, we prove in a similar way that

$$\frac{\sigma^2\left[D_{l^+}(G^c)\right]}{\sigma^2\left[D_{l^+}(G)\right]} = O(N^{-1}) \to 0.$$

Appendix C: Proof of Theorem 2

First, we note from (13) that

$$\max\rho(G^c(N,p)) = -\frac{p}{1-p}\min\rho(G(N,p)) - \frac{2}{(N-2)(1-p)}.$$

Let $R_N(p) = \max\rho(N,p) + \min\rho(N,p)$. From (13), it follows that, $R_N(p) = -\frac{p}{1-p}R_N(1-p) - \frac{4}{(N-2)(1-p)}$. By setting $p = \frac{1}{2}$, one obtains $R_N(\frac{1}{2}) = -R_N(\frac{1}{2}) - \frac{8}{N-2}$, showing that $R_N(\frac{1}{2}) = -\frac{4}{N-2}$.

The link density $p = \frac{L}{\binom{N}{2}} \in \mathbb{Q}$ is a rational number, which tends to a real number when $N \to \infty$. Assume that $\max\rho(N,p)$ is differentiable with respect to p, then so are $\min\rho(N,p)$ and $R_N(p)$. Thus,

$$\frac{d^n R_N(p)}{dp^n} = \frac{d^n}{dp^n}\left(-\frac{p}{1-p}R_N(1-p) - \frac{4}{(N-2)(1-p)}\right).$$

By applying Leibniz' rule, we have for $n \geq 1$

$$\frac{d^n}{dp^n}\left(-\frac{p}{1-p}R_N(1-p)\right) = -\sum_{j=0}^{n}\binom{n}{j}\frac{d^{n-j}}{dp^{n-j}}\left(\frac{p}{1-p}\right)\frac{d^j}{dp^j}R_N(1-p).$$

For $m > 0$, we use $\frac{d^m}{dp^m}\left(\frac{p}{1-p}\right) = \frac{d^m}{dp^m}\left(1-\frac{1}{1-p}\right) = -\frac{d^m}{dp^m}\left(\frac{1}{1-p}\right) = (-1)^m m!\,(1-p)^{-m-1}$ such that

$$\frac{d^n}{dp^n}\left(-\frac{p}{1-p}R_N(1-p)\right) = -\left(\frac{p}{1-p}\right)\frac{d^n R_N(1-p)}{dp^n} + \frac{(-1)^n n!}{(1-p)^{n+1}}\sum_{j=0}^{n-1}\frac{1}{j!}\frac{d^j R_N(1-p)}{dp^j}(1-p)^j.$$

Hence,

$$\frac{d^n R_N(p)}{dp^n} = -\left(\frac{p}{1-p}\right)\frac{d^n R_N(1-p)}{dp^n} + \frac{(-1)^n n!}{(1-p)^{n+1}}\sum_{j=0}^{n-1}\frac{1}{j!}\frac{d^j R_N(1-p)}{dp^j}(1-p)^j + \frac{(-1)^n 4(n!)}{(N-2)(1-p)^{n+1}}. \quad \text{(C.1)}$$

Setting $n = 1$ renders

$$\frac{dR_N(p)}{dp} = -\frac{p}{1-p}\frac{dR_N(1-p)}{dp} - \frac{1}{(1-p)^2}R_N(1-p) - \frac{4}{(N-2)(1-p)^2}.$$

Evaluation at $p = \frac{1}{2}$ (with $R_N(\frac{1}{2}) = -\frac{4}{N-2}$) yields $\frac{dR_N(p)}{dp}|_{p=\frac{1}{2}} = -\frac{dR_N(1-p)}{dp}|_{p=\frac{1}{2}}$, which shows that $\frac{dR_N(p)}{dp}|_{p=\frac{1}{2}} = 0$. Since $\frac{dR_N(p)}{dp}|_{p=\frac{1}{2}} = 0$, it also follows from (C.1) that $\frac{d^2R_N(p)}{dp^2}|_{p=\frac{1}{2}} = 0$ and in fact, by iteration, that $\frac{d^nR_N(p)}{dp^n}|_{p=\frac{1}{2}} = 0$. The Taylor expansion of $R_N(p)$ around $p = \frac{1}{2}$,

$$R_N(p) = \sum_{n=0}^{\infty} \frac{1}{n!} \left.\frac{d^nR_N(p)}{dp^n}\right|_{p=\frac{1}{2}} \left(p - \frac{1}{2}\right)^n = R_N\left(\frac{1}{2}\right) = -\frac{4}{N-2}$$

demonstrates that $R_N(p) = \max\rho(N,p) + \min\rho(N,p) = -\frac{4}{N-2}$. Hence, the maximum and minimum assortativity are symmetric around $\rho_D = 0$ when $N \to \infty$, in which case the assumption of differentiability with respect to p also holds. This proves Theorem 2.

Appendix D: An example of a strict disassortative class of graphs

Consider the connected graphs in which $N-2$ nodes have degree r and the two remaining nodes, 1 and 2, have degree d_1 and d_2. Thus, the basic law of the degree tells us that

$$2L = (N-2)r + d_1 + d_2.$$

There are only two configurations possible that lead to a different sum $S = \sum_{i\sim j}(d_i - d_j)^2$ in (1): (a) when node 1 and node 2 are not mutually connected and (b) when they are. In the first case,

$$S_1 = d_1(r-d_1)^2 + d_2(r-d_2)^2,$$

and in the second case,

$$S_2 = (d_1-d_2)^2 + (d_1-1)(r-d_1)^2 + (d_2-1)(r-d_2)^2 = S_1 + (d_1-d_2)^2 - (r-d_1)^2 - (r-d_2)^2.$$

Now,

$$(d_1-d_2)^2 - (r-d_1)^2 - (r-d_2)^2 = -2(r-d_1)(r-d_2)$$

such that

$$S_2 = S_1 - 2(r-d_1)(r-d_2). \qquad \text{(D.1)}$$

The basic law of the degree $2L = Nr + (d_1 - r) + (d_2 - r)$ allows us to eliminate d_2,

$$S_2 = S_1 + 2(r-d_1)(2L - Nr) + 2(r-d_1)^2. \qquad \text{(D.2)}$$

If $r > d_1$, then it follows from (D.2) that $S_2 > S_1$ and, further from (D.1), that then $r < d_2$. If $r = d_1$, then $S_2 = S_1$. If $r < d_1$ and $r < d_2$ or $r > d_1$ and $r > d_2$, then (D.1) shows that $S_2 < S_1$.

After choosing the S_1 configuration, we rewrite (1) as

$$\rho_D = \frac{V - S_1}{V}.$$

The denominator V in (1) is, with

$$\sum_{i=1}^{N} d_i^2 = (N-2)r^2 + d_1^2 + d_2^2$$

$$\sum_{i=1}^{N} d_i^3 = (N-2)r^3 + d_1^3 + d_2^3$$

equal to

$$V = \sum_{i=1}^{N} d_i^3 - \frac{1}{2L}\left(\sum_{i=1}^{N} d_i^2\right)^2 = (N-2)r^3 + d_1^3 + d_2^3 - \frac{\left((N-2)r^2 + d_1^2 + d_2^2\right)^2}{2L}.$$

Hence,

$$S_1 - V = d_1(r-d_1)^2 + d_2(r-d_2)^2 - (N-2)r^3 - d_1^3 - d_2^3 + \frac{\left((N-2)r^2 + d_1^2 + d_2^2\right)^2}{2L}$$

from which

$$2L(S_1 - V) = \left((N-2)r^2 + d_1^2 + d_2^2 - rL\right)^2 + rL\left\{2d_1(r-d_1) + 2d_2(r-d_2) - rL\right\}.$$

Using $2L = (N-2)r + d_1 + d_2$ yields, after some tedious manipulations,

$$2L(S_1 - V) = \left\{d_1^2 + d_2^2 - r(d_1 + d_2)\right\}^2.$$

In conclusion, $S_1 - V \geq 0$ and only zero if $d_1 = d_2 = r$. Hence, since $V \geq 0$ (as shown in [3,11] and since $\rho_D = (V - S_1)/V$, we conclude that $\rho_{D1} < 0$. If $S_2 > S_1$, then $S_2 - V > 0$ such that we find a strict disassortative class. The analysis above shows that this happens if $d_1 < r < d_2$.

Appendix E: Table of assortativities for complex networks

Table E.1. Various real-world networks whose maximum and minimum assortativities were computed heuristically by greedy degree-preserving rewiring. The computation of the absolute maximum and minimum assortativity is possible as explained in [3], but it is computationally rather expensive. Although the heuristic algorithm cannot guarantee to find the optimal assortativity results, it achieves results that are close to that of the exact algorithm.

#	Name	N	L	$E[D]$	ρ_0	$\rho_{\min}$	$\rho_{\max}$	$\Delta\rho$
	Proteins							
1	1AOR	97	212	4.37	0.412	−0.959	0.955	1.91
2	1a4j	95	213	4.48	0.129	−0.959	0.992	1.95
3	1atn	5015	5128	2.05	−0.453	−0.778	0.977	1.75
4	1eaw	53	123	4.64	0.209	−0.952	0.965	1.92
5	3cro	1856	1966	2.12	−0.495	−0.842	0.979	1.82
	Software call graphs							
6	AbiWord	1093	1765	3.23	−0.0777	−0.33	0.309	0.639
7	Digital Material	187	269	2.88	−0.179	−0.516	0.235	0.751
8	MySql	1500	4202	5.60	−0.0825	−0.21	0.0521	0.262
9	VTK	786	1370	3.49	−0.191	−0.418	0.309	0.727
10	XMMS	1097	1894	3.45	−0.0809	−0.627	0.848	1.48
	Food webs							
11	Everglades	69	880	25.5	−0.298	−0.584	−0.0462	0.538
12	Florida	128	2075	32.4	−0.112	−0.565	0.196	0.761
13	St. Marks	54	350	13.0	−0.232	−0.467	−0.0361	0.431
	Telecommunications networks							
14	ARPANET80	71	86	2.42	−0.261	−0.824	0.845	1.67
15	Surfnet	65	111	3.42	0.229	−0.916	0.950	1.87
	Electronic circuits							
16	s208	122	189	3.10	−0.00201	−0.729	0.845	1.57
17	s420	252	399	3.17	−0.00591	−0.657	0.783	1.44
18	s838	512	819	3.20	−0.03	−0.483	0.567	1.05
	Peer-to-peer networks							
19	Gnutella 1	737	803	2.18	−0.193	−0.582	0.848	1.43
20	Gnutella 2	1568	1906	2.43	−0.0946	−0.122	−0.0211	0.101
21	Gnutella 3	435	459	2.11	−0.33	−0.351	−0.141	0.210
22	Gnutella 4	653	738	2.26	−0.246	−0.259	−0.168	0.0913
	Power grids							
23	Western European power grid level 2 AL	3690	4206	2.28	0.0649	−0.259	0.958	1.22
24	Western European power grid level 3 AL	756	786	2.08	0.00648	−0.273	0.497	0.770
25	Western US power grid	4941	6594	2.67	0.00346	−0.695	0.975	1.67
	Miscellaneous networks							
26	American football contest network	115	613	10.7	0.162	−0.713	0.924	1.64
27	C. elegans neural network	297	2148	14.5	−0.163	−0.449	0.149	0.598
28	Dolphin social network	62	159	5.13	−0.0436	−0.979	0.895	1.87
29	Dutch football player co-appearance network	685	10310	30.1	−0.0634	−0.95	0.897	1.85
30	Les Miserable co-appearance network	77	254	6.60	−0.165	−0.746	0.202	0.949
31	Network science collaboration network	1461	2742	3.75	0.462	−0.638	0.935	1.57
32	Western European railway network level 2 AL	697	785	2.25	0.0954	−0.642	0.963	1.61
33	Word adjacency network – Japanese texts	2704	7998	5.92	−0.259	−0.321	−0.204	0.117
34	Word adjacency network – David Copperfield	112	425	7.59	−0.129	−0.598	0.147	0.745

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