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Influence of Assortativity and Degree-preserving Rewiring on the Spectra of Networks

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Abstract. Newman's measure for (dis)assortativity, the linear degree correlation coefficient ρ_D, is reformulated in terms of the total number N_k of walks in the graph with k hops. This reformulation allows us to derive a new formula from which a degree-preserving rewiring algorithm is deduced, that, in each rewiring step, either increases or decreases ρ_D conform our desired objective. Spectral metrics (eigenvalues of graph-related matrices), especially, the largest eigenvalue λ_1 of the adjacency matrix and the algebraic connectivity μ_{N-1} (second-smallest eigenvalue of the Laplacian) are powerful characterizers of dynamic processes on networks such as virus spreading and synchronization processes. We present various lower bounds for the largest eigenvalue λ_1 of the adjacency matrix and we show, apart from some classes of graphs such as regular graphs or bipartite graphs, that the lower bounds for λ_1 increase with ρ_D. An new upper bound for the algebraic connectivity μ_{N-1} decreases with ρ_D. Applying the degree-preserving rewiring algorithm to various real-world networks illustrates that (a) assortative degree-preserving rewiring increases λ_1, but decreases μ_{N-1}, even leading to disconnectivity of the networks in many disjoint clusters and that (b) disassortative degree-preserving rewiring decreases λ_1, but increases the algebraic connectivity, at least in the initial rewirings.

1 Introduction

"Mixing" in complex networks [14] refers to the tendency of network nodes to connect preferentially to other nodes with either similar or opposite properties. Mixing is computed via the correlations between the properties, such as the degree, of nodes in a network. Networks, where high-degree nodes preferentially connect to other high-degree nodes, are called *assortative*, whereas networks, where high-degree nodes connect to low-degree nodes, are called *disassortative*. The degree correlation is widely studied after it was realized that the degree distribution alone provides a far from sufficient characterization of complex networks. Networks with a same degree distribution may still differ significantly in various topological features (as we will also show in this paper). A stronger confinement than a same degree distribution are networks with a same – apart from a possible node relabelling – degree vector $d^T = [d_1, d_2, ..., d_N]$, where d_j is the degree of node j. Also "same degree vector" networks may possess widely different topological properties. Consequently, degree correlation related investigations have been performed along various axes: a) models to generate networks with given degree correlation have been developed [13][2]; b) the effect of degree correlation on topological properties is studied in [25][12], and c) the influence of degree correlation in dynamic processes on networks such as the epidemic spreading [5] and on percolation phenomena [16] have been targeted. Relations between degree correlation and other topological or dynamic features are examined experimentally [25] or in a specific network model [16][5]. "Local" assortativity is proposed in [17]. Analytic insight in degree correlations in an arbitrary network remains far from well understood. In this work, we explore the influence of the degree correlation on spectra of networks, which well capture both topological properties [23] and dynamic processes [4] on the network.

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. The adjacency spectrum of a graph is the set of eigenvalues of the adjacency matrix, $\lambda_N \leq \lambda_{N-1} \leq \cdots \leq \lambda_1$, where λ_1 is called the spectral radius. The Laplacian matrix of G with N nodes is an $N \times N$ symmetric matrix $Q = \Delta - A$, where $\Delta = \text{diag}(d_i)$ and d_i is the degree of node $i \in \mathcal{N}$. The set of N eigenvalues of the Laplacian matrix $\mu_N = 0 \leq \mu_{N-1} \leq ... \leq \mu_1$ is called the Laplacian spectrum of G. The theory of the spectra of graphs provides many beautiful results [23]. Recently, modern network theory has been integrated with dynamic system's theory to understand how the network topology can predict dynamic processes such as synchronization or virus spread taking place on networks. The SIS (susceptable-infected-susceptable) virus spreading [24] and the Kuramoto type of synchronization process of coupled oscillators [18] have been characterized on a given, but general, network topology. Both these dynamic and non-linear processes feature a phase transition, that specifies the onset of a remaining fraction of infected nodes and of locked oscillators, respectively. The more curious aspect is that each of the phase transitions in these different processes occurs at an effective spreading rate τ_c and coupling strength g_c respectively, that is proportional to $1/\lambda_1$. In addition, dynamic processes on graphs converge towards their steady-state, in most cases, exponentially fast in time and with a time-constant related to the spectral gap (difference between λ_1 and λ_2). Connectivity and the number of disjoint clusters in G follows from the algebraic connectivity (second-smallest eigenvalue of the Laplacian) and the number of smallest Laplacian eigenvalues that are zero [23]. Hence, these spectral metrics (eigenvalues of graph-related matrices), especially, the largest eigenvalue λ_1 of the adjacency matrix and the algebraic connectivity μ_{N-1}, are powerful characterizers of dynamic processes on graphs.

The present paper starts with a reformulation of the linear degree correlation coefficient ρ_D, introduced by Newman [14, eq (21)], in terms of the total number N_k of walks in the graph with k hops. This reformulation allows us to derive a new formula from which a degree-preserving rewiring algorithm is deduced, that, in each rewiring step, either increases or decreases ρ_D conform the desired objective. Thus, we construct a sequence of degree-preserving rewirings that monotonously in- or decreases the linear degree correlation coefficient ρ_D, or equivalently, that increases the assortativity or disassortativity of G. Next, we present various lower bounds for λ_1 and we show, apart from some classes of graphs such as regular graphs or bipartite graphs, that lower bounds for λ_1 increase with ρ_D. We derive an upper bound for the algebraic connectivity μ_{N-1} that decreases with ρ_D. Then, as an example, we apply the degree-preserving rewiring algorithm to a real-world network, the USA air transportation network, and compute in each rewiring the entire adjacency and Laplacian spectrum. A major finding, also observed in other real-world networks that we have rewired, is that, increasing λ_1 by increasing the assortativity, relatively rapidly leads to disconnectivity, while increasing disassortativity seems to increase the algebraic connectivity μ_{N-1}, thus the topological robustness.

2 Reformulation of Newman's definition

Here, we study the degree mixing in undirected graphs. Generally, the linear correlation coefficient between two random variables X and Y is defined [22, p. 30] as

$$\rho(X,Y) = \frac{E[XY] - \mu_X \mu_Y}{\sigma_X \sigma_Y} \tag{1}$$

where $\mu_X = E[X]$ and $\sigma_X = \sqrt{\operatorname{Var}[X]}$ are the mean and standard deviation of the random variable X, respectively. Newman [14, eq. (21)] has expressed the linear degree correlation coefficient of a graph as

$$\rho_D = \frac{\sum_{xy} xy\,(e_{xy} - a_x b_y)}{\sigma_a \sigma_b} \tag{2}$$

where e_{xy} is the fraction of all links that connect the nodes with degree x and y and where a_x and b_y are the fraction of links that start and end at nodes with degree x and y, satisfying the following three conditions

$$\sum_{xy} e_{xy} = 1,\ a_x = \sum_y e_{xy} \text{ and } b_y = \sum_x e_{xy}$$

When $\rho_D > 0$, the graph possesses assortative mixing, a preference of high-degree nodes to connect to other high-degree nodes and, when $\rho_D < 0$, the graph features disassortative mixing, where high-degree nodes are connected to low-degree nodes.

The translation of (2) into the notation of random variables is presented as follows. Denote by D_i and D_j the node degree of two *connected* nodes i and j in an undirected graph with N nodes. In fact, we are interested in the degree of nodes at both sides of a link, without taking the link, that we are looking at, into consideration. As Newman [14] points out, we need to consider the number of excess links at both sides, hence, the degree $D_{l^+} = D_i - 1$ and $D_{l^-} = D_j - 1$, where the link l has a start at $l^+ = i$ and an end at $l^- = j$. The linear correlation coefficient of those excess degrees is

$$\rho\left(D_{l^+}, D_{l^-}\right) = \frac{E\left[D_{l^+}D_{l^-}\right] - E\left[D_{l^+}\right]E\left[D_{l^-}\right]}{\sigma_{D_{l^+}}\sigma_{D_{l^-}}}$$
$$= \frac{E\left[\left(D_{l^+} - E\left[D_{l^+}\right]\right)\left(D_{l^-} - E\left[D_{l^-}\right]\right)\right]}{\sqrt{E\left[\left(D_{l^+} - E\left[D_{l^+}\right]\right)^2\right]E\left[\left(D_{l^-} - E\left[D_{l^-}\right]\right)^2\right]}}$$

Since $D_{l^+} - E\left[D_{l^+}\right] = D_i - E\left[D_i\right]$, subtracting everywhere one link does not change the linear correlation coefficient, provided $D_i > 0$ (and similarly that $D_j > 0$), which is the case if there are no isolated nodes. Removing isolated nodes from the graph does not alter the linear degree correlation coefficient (2). Hence, we can assume that the graph has no zero-degree nodes. In summary, the linear degree correlation coefficient is

$$\rho\left(D_{l^+}, D_{l^-}\right) = \rho\left(D_i, D_j\right) = \frac{E\left[D_iD_j\right] - \mu_{D_i}^2}{E\left[D_i^2\right] - \mu_{D_i}^2} \tag{3}$$

We now proceed by expressing $E\left[D_iD_j\right]$, $E\left[D_i\right]$ and σ_{D_i} in the definition of $\rho\left(D_{l^+}, D_{l^-}\right) = \rho\left(D_i, D_j\right)$ for undirected graphs in terms of more appropriate quantities of algebraic graph theory. First, we have that

$$E\left[D_iD_j\right] = \frac{1}{2L}\sum_{i=1}^{N}\sum_{j=1}^{N} d_i d_j a_{ij} = \frac{d^T A d}{2L}$$

where d_i and d_j are the elements in the degree vector $d^T = [d_1, d_2, ..., d_N]$, and a_{ij} is the element of the symmetric adjacency matrix A, that expresses $\{0, 1\}$ connectivity between nodes i and j. The quadratic form $d^T A d$ can be written in terms of the total number $N_k = u^T A^k u$ of walks with k hops (see e.g. [23]), where u is the all-one vector. Since $d = Au$, $d^T A d$ equals $N_3 = u^T A^3 u$, the total number of walks with length equal to 3 hops, which is called the s metric in [12]. The average μ_{D_i} and μ_{D_j} are the mean node degree of the two connected nodes i and j, respectively, and not the mean of the degree D of a random node, which equals $E\left[D\right] = \frac{2L}{N}$. Thus,

$$\mu_{D_i} = \frac{1}{2L}\sum_{i=1}^{N}\sum_{j=1}^{N} d_i a_{ij} = \frac{1}{2L}\sum_{i=1}^{N} d_i \sum_{j=1}^{N} a_{ij}$$
$$= \frac{1}{2L}\sum_{i=1}^{N} d_i^2 = \frac{d^T d}{2L}$$

while

$$\mu_{D_j} = \frac{1}{2L}\sum_{i=1}^{N}\sum_{j=1}^{N} d_j a_{ij} = \mu_{D_i}$$

The variance $\sigma_{D_i}^2 = \mathrm{Var}[D_i] = E\left[D_i^2\right] - \mu_{D_i}^2$ and

$$E\left[D_i^2\right] = \frac{1}{2L}\sum_{i=1}^{N}\sum_{j=1}^{N} d_i^2 a_{ij} = \frac{1}{2L}\sum_{i=1}^{N} d_i^3 = E\left[D_j^2\right]$$

After substituting all terms into the expression (3) of the linear degree correlation, we obtain, with $N_1 = 2L$ and $N_2 = d^T d$, our reformulation of Newman's definition (2) in terms of N_k,

$$\rho_D = \rho\left(D_i, D_j\right) = \frac{N_1 N_3 - N_2^2}{N_1 \sum_{i=1}^{N} d_i^3 - N_2^2} \tag{4}$$

The crucial understanding of (dis)assortativity lies in the total number N_3 of walks with 3 hops compared to those with 2 hops, N_2, and one hop, $N_1 = 2L$.

3 Discussion of (4)

Fiol and Garriga [8] have shown that the total number $N_k = u^T A^k u$ of walks of length k is upper bounded by

$$N_k \leq \sum_{j=1}^{N} d_j^k$$

with equality only if $k \leq 2$ and, for all k, only if the graph is regular (i.e., $d_j = r$ for any node j). Hence, (4) shows that only if the graph is regular, $\rho_D = 1$, implying that maximum assortativity is only possible in regular graphs[1]. Since the variance of the degrees at one side of an arbitrary link

$$\sigma_{D_i}^2 = \frac{1}{N_1} \sum_{i=1}^{N} d_i^3 - \left(\frac{N_2}{N_1} \right)^2 \geq 0 \tag{5}$$

the sign of $N_1 N_3 - N_2^2$ in (4) distinguishes between assortativity ($\rho_D > 0$) and disassortativity ($\rho_D < 0$). Using the Laplacian matrix, Fiol and Garriga [8] show that

$$\sum_{i=1}^{N} d_i^3 - N_3 = \sum_{i \sim j} (d_i - d_j)^2 = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} a_{ij} (d_i - d_j)^2 \tag{6}$$

which is the sum over all links of the square of the differences of the degrees at both sides of a link $l = i \sim j$. Using (6), the degree correlation (4) can be rewritten as

$$\rho_D = 1 - \frac{\sum_{i \sim j} (d_i - d_j)^2}{\sum\limits_{i=1}^{N} d_i^3 - \frac{1}{2L} \left(\sum\limits_{i=1}^{N} d_i^2 \right)^2} \tag{7}$$

The graph is zero assortative ($\rho_D = 0$) if

$$N_2^2 = N_1 N_3 \tag{8}$$

In Appendix A, we show that the connected Erdős-Rényi random graph $G_p(N)$ is zero-assortative for all N and link density $p > p_c$, where p_c is the disconnectivity threshold (see [22, p. 329-338]). Asymptotically for large N, the Barabási-Albert power law graph is zero-assortative as shown in [15].

Perfect disassortativity ($\rho_D = -1$ in (4)) implies that

$$N_2^2 = \frac{N_1}{2} \left(N_3 + \sum_{i=1}^{N} d_i^3 \right) \tag{9}$$

For a complete bipartite graph[2] $K_{m,n}$, we have that

$$\sum_{i \sim j} (d_i - d_j)^2 = mn (n - m)^2, \sum_{i=1}^{N} d_i^3 = nm \left(n^2 + m^2 \right)$$

$$\text{and } \sum_{i=1}^{N} d_i^2 = nm (n + m)$$

such that (7) becomes $\rho_D = -1$, provided $m \neq n$. Hence, any complete bipartite graph $K_{m,n}$ (irrespective of its size and structure (m, n), except for the regular graph variant where $m = n$) is perfectly disassortative. The perfect disassortativity of complete bipartite graphs is in line with the definition of disassortativity, because each node has only links to nodes of a different set with different properties. Nevertheless, the fact that all complete bipartite graphs $K_{m,n}$ with $m \neq n$ have $\rho_D = -1$, even those with

[1] Notice that the definition (4) is inadequate (due to a zero denominator and numerator) for a regular graph with degree r because $N_{k \text{ regular graph}} = N r^k$. For regular graphs where $\sum_{i=1}^{N} d_i^3 = N_3$, the perfect disassortativity condition (9) becomes $N_2^2 = N_1 N_3$, which is equal to the zero assortativity condition (8). Of course, $\rho_{\text{regular graph}} = 1$, since all degrees are equal and thus perfectly correlated.

[2] The complete bipartite graph $K_{m,n}$ consists of two sets $\mathcal{M}$ and $\mathcal{N}$ with $m = |\mathcal{M}|$ and $n = |\mathcal{N}|$ nodes respectively, where each node of one set is connected to all other nodes of the other set. There are no links between nodes of a same set. More properties are deduced in [23].

nearly the same degrees $m = n \pm 1$ and thus close to regular graphs typified by $\rho_D = 1$, shows that assortativity and disassortativity of a graph is not easy to predict. It remains to be shown that the complete bipartite graphs $K_{m,n}$ with $m \neq n$ are the only perfect disassortative class of graphs.

There is an interesting relation between the linear degree correlation coefficient ρ_D of the graph G and the variance of the degree of a node in the corresponding line graph $l(G)$. The line graph $l(G)$ of the graph $G(N,L)$ has as set of nodes the links of G and two nodes in $l(G)$ are adjacent if and only if they have, as links in G, exactly one node of G in common. The l-th component of the $L \times 1$ degree vector in the line graph $l(G)$ (see [23]) is $\left(d_{l(G)}\right)_l = d_i + d_j - 2$, where node i and j are connected by link $l = i \sim j$. The variance of the degree $D_{l(G)}$ of a random node in the line graph equals

$$\operatorname{Var}\left[D_{l(G)}\right] = E\left[(D_i + D_j)^2\right] - \left(E\left[D_i + D_j\right]\right)^2$$

which we rewrite as

$$\operatorname{Var}\left[D_{l(G)}\right] = 2\left(E\left[D_i^2\right] - \mu_{D_i}^2 + E\left[D_i D_j\right] - \mu_{D_i}^2\right)$$

Using (3), we arrive at

$$\begin{aligned}\operatorname{Var}\left[D_{l(G)}\right] &= 2\left(1+\rho_D\right)\left(E\left[D_i^2\right] - \mu_{D_i}^2\right) \\ &= \left(1+\rho_D\right)\operatorname{Var}\left[D_i\right] \\ &= 2\left(1+\rho_D\right)\left(\frac{1}{N_1}\sum_{i=1}^N d_i^3 - \left(\frac{N_2}{N_1}\right)^2\right) \qquad (10)\end{aligned}$$

Curiously, the expression (10) shows for perfect disassortative graphs ($\rho_D = -1$) that $\operatorname{Var}\left[D_{l(G)}\right] = 0$. The latter means that $l(G)$ is then a regular graph, but this does not imply that the original graph G is regular. Indeed, if G is regular, then $l(G)$ is also regular as follows from l-th component of the degree vector, $\left(d_{l(G)}\right)_l = d_i + d_j - 2$. However, the reverse is not necessarily true: it is possible that $l(G)$ is regular, while G is not, as shown above, for complete bipartite graphs $K_{m,n}$ with $m \neq n$ that are not regular. In summary, in both extreme cases $\rho_D = -1$ and $\rho_D = 1$, the corresponding line graph $l(G)$ is a regular graph.

4 Relation between graph spectra and ρ_D

The largest eigenvalue λ_1 of the adjacency matrix A of a graph as well as the algebraic connectivity μ_{N-1}, introduced by Fiedler [7], are important characterizers of a graph. Here, we present a new lower bound for λ_1 and upper bound of μ_{N-1} in terms of the linear degree coefficient ρ_D.

In [23, Chapter 3], we show, for all integers $k \geq 1$, that

$$\lambda_1 \geq \left(\frac{N_{2k}}{N}\right)^{1/(2k)} \geq \left(\frac{N_k}{N}\right)^{1/k}$$

from which $\lim_{k\to\infty}\left(\frac{N_k}{N}\right)^{1/k} = \lambda_1$. We obtain the classical lower bound for $k = 1$,

$$\lambda_1 \geq \frac{N_1}{N} = \frac{2L}{N} = E[D] \qquad (11)$$

and for $k = 2$,

$$\lambda_1 \geq \sqrt{\frac{N_2}{N}} = \sqrt{\frac{1}{N}\sum_{k=1}^N d_k^2} = \frac{2L}{N}\sqrt{1 + \frac{\operatorname{Var}[D]}{\left(E[D]\right)^2}} \qquad (12)$$

For $k = 3$ and using (4), we obtain

$$\lambda_1^3 \geq \frac{N_3}{N} = \frac{1}{N}\left(\rho_D\left(\sum_{i=1}^N d_i^3 - \frac{N_2^2}{N_1}\right) + \frac{N_2^2}{N_1}\right) \qquad (13)$$

The inequality (13) with (5) shows that the lower bound for the largest eigenvalue λ_1 of the adjacency matrix A

is strictly increasing in the linear degree correlation coefficient ρ_D (except for regular graphs). Given the degree vector d is constant, inequality (13) shows that the largest eigenvalue λ_1 is obtained in case we succeed to increase the assortativity of the graph by degree-preserving rewiring, which is discussed in Section 5.

A related bound, deduced from Rayleigh's inequality $\lambda_1 \geq \frac{y^T A y}{y^T y}$ by choosing the vector $y = A^m u$, where u is the all-one vector and m is a non-zero integer, is

$$\lambda_1 \geq \frac{u^T A^{2m+1} u}{u^T A^{2m} u} = \frac{N_{2m+1}}{N_{2m}} \tag{14}$$

The case $m = 1$ in (14), $\lambda_1 \geq \frac{N_3}{N_2}$, already appeared as an approximation in [19] of the largest adjacency eigenvalue λ_1, which, again in view of (4), is a perfect linear function of ρ_D. Finally, we present the new, optimized bound, derived in [23, Chapter 3],

$$\lambda_1 \geq \frac{N_0 N_3 - N_1 N_2 + R}{2\left(N_0 N_2 - N_1^2\right)} \tag{15}$$

where

$$R = \sqrt{N_0^2 N_3^2 - 6 N_0 N_1 N_2 N_3 - 3 N_1^2 N_2^2 + 4\left(N_1^3 N_3 + N_0 N_2^3\right)}$$

Fig. 1 illustrates how the largest eigenvalue λ_1 of the Barabasi-Albert power-law graph evolves as a function of the linear degree correlation coefficient ρ_D, that can be changed by degree-preserving rewiring. The lower bound (15) clearly outperforms the lower bound[3] (13). Especially in degree-preserving rewiring, where N_0, N_1 and N_2 are constant, the complex looking, but superior formula (15) becomes manageable, because only N_3 changes with ρ_D.

[3] Especially for strong negative ρ_D, we found – very rarely though – that (15) can be slightly worse than (12).

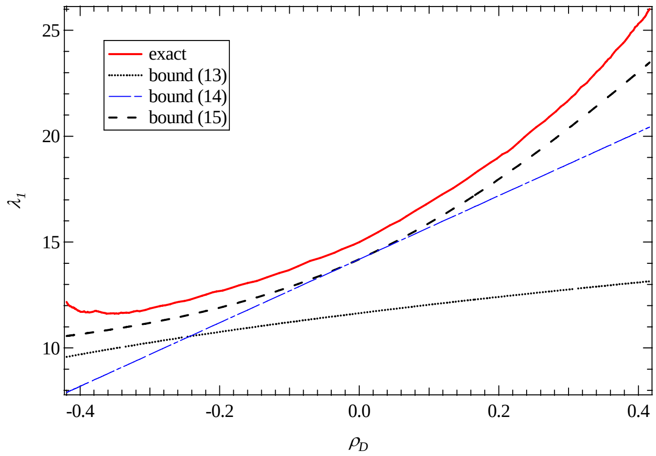

Fig. 1. The largest eigenvalue λ_1 of the Barabasi-Albert power-law graph with $N = 500$ nodes and $L = 1960$ links versus the linear degree correlation coefficient ρ_D. Various lower bounds are plotted: bound (13), bound (15) and bound (14) for $m = 1$. The corresponding classical lower bound (11) is 7.84, while the lower bound (12) is 10.548.

The Rayleigh principle (see e.g. [23,7]) provides an upper bound for the second-smallest eigenvalue μ_{N-1} of the Laplacian $Q = \text{diag}(d_j) - A$ as

$$\mu_{N-1} \leq \frac{\sum_{l\in\mathcal{L}} \left(g\left(l^+\right) - g\left(l^-\right)\right)^2}{\sum_{n\in\mathcal{N}} g^2(n) - \frac{1}{N}\left(\sum_{u\in\mathcal{N}} g(u)\right)^2}$$

where $g(n)$ is any non-constant function. Let $g(n) = d_n$, the degree of a node n, then

$$\mu_{N-1} \leq \frac{\sum_{l\in\mathcal{L}} \left(d_{l^+} - d_{l^-}\right)^2}{\sum_{j=1}^N d_j^2 - \frac{1}{N}\left(\sum_{j=1}^N d_j\right)^2} = \frac{\sum_{l\in\mathcal{L}} \left(d_{l^+} - d_{l^-}\right)^2}{N \text{Var}[D]}$$

After introducing (7), we find for any non-regular graph

$$\mu_{N-1} \leq (1-\rho_D) \frac{\sum_{i=1}^N d_i^3 - \frac{1}{2L}\left(\sum_{i=1}^N d_i^2\right)^2}{\sum_{j=1}^N d_j^2 - \frac{1}{N}\left(\sum_{j=1}^N d_j\right)^2} \tag{16}$$

$$= (1-\rho_D) \frac{E[D]\,E\left[D^3\right] - \left(E\left[D^2\right]\right)^2}{E[D]\,\text{Var}[D]} \tag{17}$$

which is an upper bound for the algebraic connectivity μ_{N-1} in terms of the linear correlation coefficient of the degree ρ_D. In degree-preserving rewiring, the fraction in (16), that is always positive, is unchanged and we observe that the upper bound decreases linearly in ρ_D.

5 Degree-preserving rewiring

In degree-preserving rewiring, links in a graph are rewired while maintaining the node degrees unchanged. This means that the degree vector d is constant and, consequently, that $N_1 = \sum_{i=1}^{N} d_i, N_2 = \sum_{i=1}^{N} d_i^2$ and $\sum_{i=1}^{N} d_i^3$ do not change during degree-preserving rewiring, only N_3 does, and by (4), also the (dis)assortativity ρ_D.

A degree-preserving rewiring changes only the term $\sum_{i\sim j} (d_i - d_j)^2$ in (7), which allows us to understand how a degree-preserving rewiring operation changes the linear degree correlation ρ_D. Each step in a degree-preserving random rewiring consists of first randomly selecting two links $i \sim j$ and $k \sim l$ associated with the four nodes i, j, k, l. Next, the links can be rewired either into $i \sim k$ and $j \sim l$ or into $i \sim l$ and $j \sim k$.

Lemma 1 *Given a graph in which two links are degree-preservingly rewired. We order the degree of the four involved nodes as $d_{(1)} \geq d_{(2)} \geq d_{(3)} \geq d_{(4)}$. The two links are associated with the 4 nodes $n_{d_{(1)}}, n_{d_{(2)}}, n_{d_{(3)}}$ and $n_{d_{(4)}}$ only in one of the following three ways: a) $n_{d_{(1)}} \sim n_{d_{(2)}}$, $n_{d_{(3)}} \sim n_{d_{(4)}}$, b) $n_{d_{(1)}} \sim n_{d_{(3)}}$, $n_{d_{(2)}} \sim n_{d_{(4)}}$, and c) $n_{d_{(1)}} \sim n_{d_{(4)}}$, $n_{d_{(2)}} \sim n_{d_{(3)}}$. The corresponding linear degree correlation introduced by these three possibilities obeys $\rho_a \geq \rho_b \geq \rho_c$.*

Proof: In these three ways of placing the two links, the degree of each node remains the same. According to definition (7), the linear degree correlation is determined only by $\varepsilon = -\sum_{i\sim j} (d_i - d_j)^2$. Thus, the relative degree correlation difference between (a) and (b) is

$$\begin{aligned}
\varepsilon_a - \varepsilon_b &= -\left(d_{(1)} - d_{(2)}\right)^2 - \left(d_{(3)} - d_{(4)}\right)^2 \\
&\quad + \left(d_{(1)} - d_{(3)}\right)^2 + \left(d_{(2)} - d_{(4)}\right)^2 \\
&= 2(d_{(2)} - d_{(3)})(d_{(1)} - d_{(4)}) \geq 0
\end{aligned}$$

since the rest of the graph remains the same in all three cases. Similarly,

$$\varepsilon_a - \varepsilon_c = 2(d_{(2)} - d_{(4)})(d_{(1)} - d_{(3)}) \geq 0$$
$$\varepsilon_b - \varepsilon_c = 2(d_{(1)} - d_{(2)})(d_{(3)} - d_{(4)}) \geq 0$$

These three inequalities complete the proof. □

A direct consequence of Lemma 1 is that we can now design a rewiring rule that increases or decreases the linear degree correlation ρ_D of a graph. We define *degree-preserving assortative random rewiring* as follows: Randomly select two links associated with four nodes and then rewire the two links such that as in a) the two nodes with the highest degree and the two lowest-degree nodes are connected. If any of the new links exists before rewiring, discard this step and a new pair of links is randomly selected. Alternatively, we could select two links for which $\sum_{i\sim j} (d_i - d_j)^2$ is highest and rewire them such that the highest-degree nodes are connected and the lowest-degree nodes are connected. Similarly, the procedure for *degree-preserving disassortative random rewiring* is: Randomly select two links associated with four nodes and then rewire the two links such that as in c) the highest-degree node and the lowest-degree node are connected, while also the remaining two nodes are linked provided the new links do not exist before rewiring. Lemma 1 shows that the degree-preserving assortative (disassortative) rewiring operations increase (decrease) the degree correlation of a graph.

Degree-preserving rewiring is an interesting tool to modify a graph in which resources of the nodes are constrained. For example, the number of outgoing links in a router [3] as well as the number of flights at many airports per day are almost fixed. Random degree-preserving rewiring may be considered as an evolutionary process in nature.

5.1 Algorithmic considerations

In this subsection, we concentrate on the following problem:

Problem 1 Given a degree vector d consisting of N elements, find a (not necessarily connected) simple[4] graph such that the assortativity ρ_D is maximum (minimum).

Before presenting the solution, we evaluate two intuitive approaches. The first method, used in [26] and coined the stochastic approach, consists of repeating *degree-preserving assortative random rewiring* long enough. The stochastic approach stabilizes, after long enough rewiring, to some level $\tilde{\rho}_D$. Next we check all possible $\binom{L}{2}$ pairs of links whether we still can rewire a pair to increase ρ_D. If we cannot rewire any pair of links to increase ρ_D, we have definitely found a local maximum. However, this local maximum is not guaranteed to be the overall or global maximum. This can be verified by executing the stochastic approach on a same graph a number of times: each realization (including the check over all possible $\binom{L}{2}$ pairs of links) does not necessarily achieve the same maxρ_D.

[4] A simple graph is an unweighted, undirected graph containing no self-loops (links starting and ending at the same node) nor multiple links between the same pair of nodes.

The second deterministic approach attempts to find an $N \times N$ matrix A that maximizes $N_3 = d^T Ad$, while maintaining the degree vector d unchanged. Without loss of generality we can assume that the components of the degree vector d are ordered as $d_1 \geq ... \geq d_N$. The elements a_{ij} of A should be determined such that $N_3 = \sum_{j=1}^{N} \sum_{i=1}^{N} a_{ij} d_i d_j$ is maximum under the condition that $\sum_{j=1}^{N} a_{ij} = d_i$, $a_{ij} = a_{ji}$, and $a_{ii} = 0$ for all i. Let us denote the vector $c = Ad$, which has non-negative components. Recall that $d = Au$, then $N_3 = d^T c$ and $u^T c = \sum_{i=1}^{N} c_i = d^T d$ is constant (because d must be unchanged). Due to the ordering $d_1 \geq ... \geq d_N$, $d^T c = \sum_{i=1}^{N} c_i d_i$ is maximum if $c_1 \geq ... \geq c_N$. We should therefore shift as much weight as possible (of the total $\sum_{i=1}^{N} c_i$) to the left side of the vector c^T. The graph constuction method in [12] that tries to optimize $\sum_{i=1}^{N} \sum_{j=1}^{N} a_{ij} d_i d_j$, belongs to the second class. This method ranks all possible links $1 \leq l \leq \binom{N}{2}$ according to $d_{l^+} d_{l^-}$ from the highest to the lowest resulting in $l_{(1)}, l_{(2)}, \ldots, l_{(\binom{N}{2})}$. Next, the graph is constructed by including sequentially links with increasing index, but links that violate the degree vector, are excluded. Both the stochastic and deterministic approach (as deployed by Li et al. [12]) are, however, heuristic, while the problem is polynomially solvable.

Problem 1 is, in fact, an instance of the maximum-weight degree-constrained subgraph problem[5], which is polynomially solvable (e.g., see [20] and [9]). The degree-constrained subgraph problem is defined as follows:

Definition 1 *Degree-constrained subgraph problem: Given a graph $G(\mathcal{N}, \mathcal{L})$ with N nodes and L links, and a degree vector $d = d_1, ..., d_N$, find a subgraph $H(\mathcal{N}, \mathcal{L}_H)$, where $\mathcal{L}_H \subseteq \mathcal{L}$, and each node i has precisely d_i neighbors (adjacent nodes).*

The problem instance that we need to solve is to find a maximum-weight degree-constrained subgraph in the complete graph K_N, where each link from a node i to a node j is assigned a weight $d_i d_j$. By finding a maximum-weight degree-constrained subgraph H, where each node $i \in \mathcal{N}$ has precisely d_i neighbors, we obtain a subgraph of the complete graph for which all nodes obey the degree sequence, and for which $N_3 = \sum_{j=1}^{N} \sum_{i=1}^{N} a_{ij} d_i d_j$ is maximum (corresponding to a graph with highest N_3 and hence assortativity).

[5] The degree-constrained subgraph problem on its turn falls under the umbrella of b-matching. A perfect b-matching is a set of links (subgraph) that span all nodes and for which each node i has (precisely or at most) $b(i)$ adjacent links in the matching. If links are assigned weights, then the maximum-weight perfect b-matching problem is to find a perfect b-matching, for which the sum of the link weights in the matching is highest among all possible perfect b-matchings. The problem is also known as f-matching or b/f-factor and has many variations.

We end the section by considering two additional and related problems. The first problem considers the difference $\max \rho_D - \min \rho_D$ that may be regarded as a metric of a given degree vector d and that reflects the adaptivity in (dis)assortativity under degree-preserved rewiring. As shown earlier, for some graphs like regular graphs, that difference $\max\rho_D - \min\rho_D = 0$, while $\max \rho_D - \min \rho_D \leq 2$. Let $A_{\max}$ be the matrix corresponding to $\max \rho_D$ and $A_{\min}$ is the matrix corresponding to $\min \rho_D$, then $\max \rho_D - \min \rho_D = \frac{N_1(d^T(A_{\max} - A_{\min})d)}{N_1 \sum_{i=1}^{N} d_i^3 - N_2^2}$. Now, $R = A_{\max} - A_{\min}$ is an $N \times N$ matrix with elements $r_{ij} \in \{0, 1, -1\}$. The 1's (or equivalently -1's) indicate where a link is present in $A_{\max}$ and not in $A_{\min}$ (or vice versa for -1's). Consequently, given that for an undirected graph $R = R^T$ is symmetric, the maximum number of links that would need to be rewired in $A_{\min}$ to get $A_{\max}$ equals the total amount of 1's (or equivalently -1's) divided by 2. The rewiring of a link in $A_{\min}$ to a link in $A_{\max}$ corresponds to rewiring an element in R with a -1 and with a 1 (in the same row or column due to symmetry of R). Through appropriate relabeling of nodes, the number of rewirings may decrease. Unfortunately, finding the minimum number of rewirings is an NP-complete problem [3].

The problem of finding a connected graph of minimum (or maximum) weight given a degree sequence is NP-complete, since by setting all degrees to 2, the problem reduces to the NP-complete Traveling Salesman Problem [10]. However, Bienstock and Günlük have proved that "If two connected graphs have the same degree sequence, then there exists a sequence of connected intermediate graphs transforming one of them to the other" [3]. Even though we cannot efficiently compute a connected graph of highest (dis)assortativity, we can use a rewiring approach to increase (dis)assortativity, while maintaining connectivity. Hence, we would like to possess a criterion to check if a rewiring will lead to disconnectivity. In the field of dynamic graph algorithms, Eppstein et al. [6] have proposed a technique to check for connectivity in $O(\sqrt{N})$ time for each link update (four updates per rewiring), which naturally beats any standard way of checking for graph connectivity.

Fig. 2. USA air transportation network, with $N = 2179$ and $L = 31326$.

5.2 Application to the USA air transport network

As an example, we consider degree-preserving rewiring in the USA air transportation network displayed in Fig. 2, where each node is an airport and each link is a flight connection between two American airports. We are interested

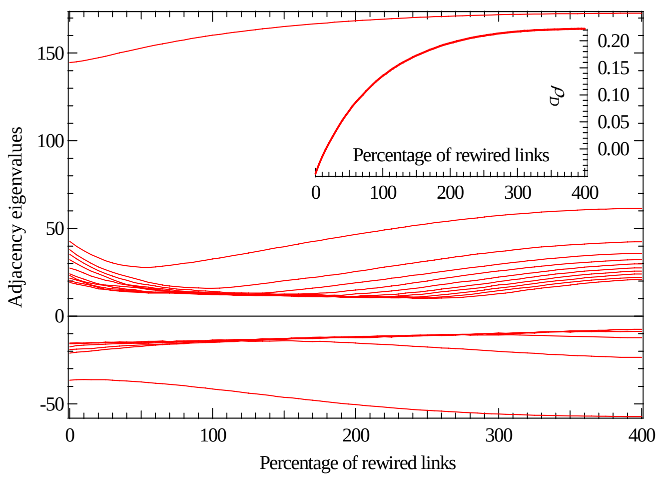

Fig. 3. The ten largest and five smallest eigenvalues of the adjacency matrix of the US airport transport network versus the percentage of rewired links. The insert shows the linear degree correlation coefficient ρ_D as function of the assortative degree-preserving rewiring.

in an infection process, where viruses are spread via airplanes from one city to another. From a topological point of view, the infection threshold $\tau_c = \frac{1}{\lambda_1}$ is the critical design parameter that we would like to have as high as possible, because an effective infection rate $\tau > \tau_c$ translates into a certain percentage of people that remains infected after sufficiently long time (see for details [24]). Since most airports operate near to full capacity, the number of flights per airport should hardly change during the re-engineering to modify the largest eigenvalue λ_1. Hence, the degree vector d should not change, which makes degree-preserving rewiring a desirable tool. Fig. 3 shows how the adjacency eigenvalues of the USA air transport network change with degree-preserving assortative rewiring. In each step of the rewiring process, only four one elements (i.e., two links) in the adjacency matrix change position. If we relabel the nodes in such a way that the link between 1 and 2 and between 3 and 4 (case a) in Lemma 1) is rewired to either case b) or c), then only a 4×4 submatrix A_4 of the adjacency matrix A in

$$A = \begin{bmatrix} A_4 & C \\ C^T & A_c \end{bmatrix}$$

is altered. The Interlacing Theorem [23, Chapter 3] states that $\lambda_{j+4}(A) \leq \lambda_j(A_c) \leq \lambda_j(A)$ for $1 \leq j \leq N-4$, which holds as well for A_r just after one degree-preserving rewiring step. Thus, apart from a few largest and smallest eigenvalues, most of the eigenvalues of A and A_r are interlaced, as observed from Fig. 3. The large bulk of the 2179 eigenvalues (not shown in Fig. 3 nor in Fig. 6) remains centered around zero and confined to the almost constant white strip between λ_{10} and λ_{N-5}. As shown above, assortative rewiring increases λ_1. Fig. 3 illustrates, in addition, that the spectral width or range $\lambda_1 - \lambda_N$ increases as well, while the spectral gap $\lambda_1 - \lambda_2$ remains high, in spite of the fact that the algebraic connectivity μ_{N-1} is small. In fact, Fig. 4 shows that μ_{N-1} decreases, in agreement with (16), and vanishes after about 10% of the link rewirings, which indicates [23, Chapter 3] that the graph is then disconnected. Fig. 4 further shows that by rewiring all links on average once (100 %), assortative degree-preserved rewiring has dissected the USA airport network into 20 disconnected clusters. Increasing the assortativity implies that high-degree and low-degree nodes are linked increasingly more to each other, which, intuitively, explains why disconnectivity in more and more clusters starts occurring during the rewiring process.

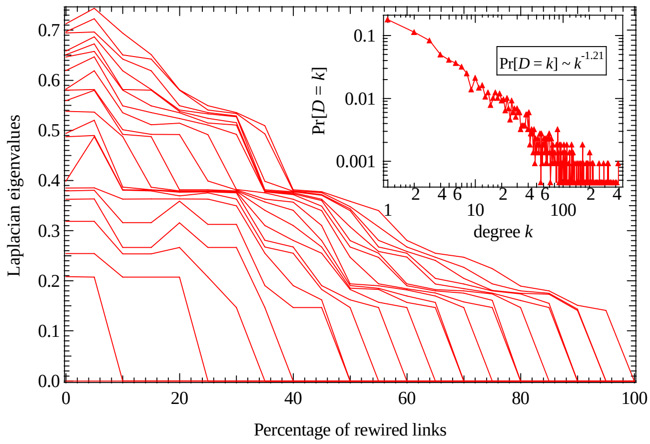

Fig. 4. The twenty smallest eigenvalues of the Laplacian matrix of the USA airport transport network versus the percentage of rewired links. The insert shows the degree distribution that is maintained in each degree-preserving rewiring step.

The opposite happens in disassortative rewiring as shown in Fig. 5: the algebraic connectivity μ_{N-1} increases during degree-preserving rewiring (up to roughly 150% rewired links) from about 0.25 to almost 1, which is the maximum possible due to $\mu_{N-1} \leq d_{\min}$, the minimum degree, and $d_{\min} = 1$ as follows from the insert in Fig. 4. Finally, Fig. 6 plots the disassortative counter part of Fig. 3: the spectral gap $\lambda_1 - \lambda_2$ reduces with the percentage of rewired links, while the spectral range $\lambda_1 - \lambda_N$ does not significantly change. The maximum difference $\max\rho_D - \min\rho_D$ is deduced from the inserts in Fig. 6 and Fig. 3 and appears to be slightly more than one, such that the adaptivity ratio in assortativity, $\frac{max\rho_D - min\rho_D}{2}$, is about 50%.

Summarizing, in order to suppress virus propagation via air transport while guaranteeing connectivity, disassortative degree-preserving rewiring is advocated, which, in return, enhances the topological robustness.

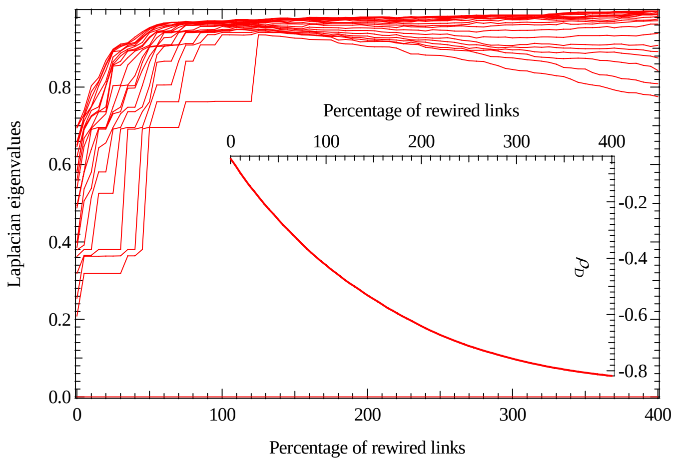

Fig. 5. The twenty smallest eigenvalues of the Laplacian versus the percentage of rewired links. The insert shows the disassortative degree-preserving rewiring.

5.3 Generalizing the observations

Degree-preserving rewirings on various other real-world complex networks confirm the above observations: (a) assortative degree-preserving rewiring increases λ_1, (b) but also decreases the algebraic connectivity μ_{N-1}, even leading to disconnectivity of the network into many clusters. (c) Disassortative degree-preserving rewiring decreases λ_1, but (d) increases the algebraic connectivity μ_{N-1} initially (roughly up to 100%) and thus strengthens the topological connectivity structure of the network.

Often, the value of a network lies in the number of its links L (relations between items), which grows as $L = O\left(N^2\right)$ in terms of the nodes at most, and in its connectivity, the ability that each node can reach each other node. A second value pillar of networking lies in positive synergetic coupling: when two nodes interact, their total impact on the network's functioning is larger than the sum of their individual functioning. Sometimes, even additional functionality is created. In order to establish positive synergy, the properties in the nodes often complement each other, which reflects disassortativity. We have shown that disassortativity decreases λ_1, implying that dynamic processes such as epidemic information spread and synchronization of coupled oscillators are "slowed-down" (as their phase-transition threshold increases). In return, disassortativity increases the algebraic connectivity μ_{N-1}, thus the ease to tear the network apart is lowered. Consequently, we argue that in most biological, infrastructural, or collaborative complex networks, disassortativity is the natural mode, because nodes with different properties connect to each other to create a network with "win-win" properties. Moreover, disassortativity favors good connectivity. Assortative networks, where nodes of the same type seek to interconnect, are less natural: either these networks are very regular and regularity is their distinguishing strength, or the nodes are selfish and only exchange with those that reward them equally, thereby excluding the lesser ones to participate in the networking.

It is interesting to mention that these inferences agree with Newman's observations [14]: Most of the biological and technical networks are disassortative, while social networks are found to be assortative.

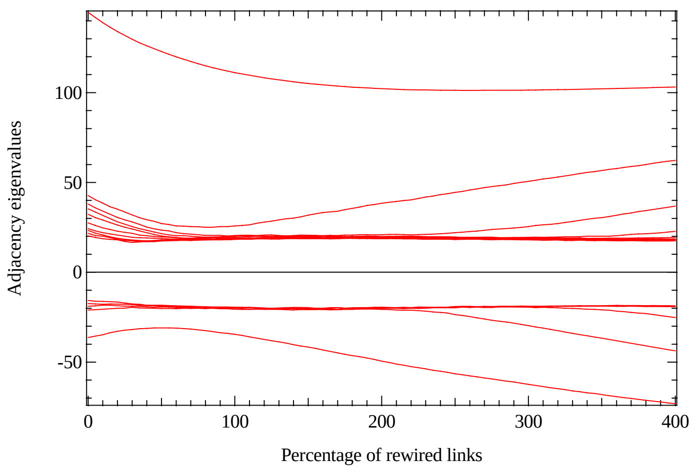

Fig. 6. The disassortative counterpart of Fig. 3.

6 Conclusions

We have reformulated the linear degree correlation coefficient ρ_D, introduced by Newman [14, eq (21)] as a measure for assortativity, in terms of the total number N_k of walks in the graph with k hops. This reformulation allows us to derive a new formula from which a degree-preserving rewiring algorithm is deduced, that, in each rewiring step, either increases or decreases ρ_D. We have investigated the degree-preserving rewiring problem in networks with a same degree vector, and presented a solution that finds the maximum assortativity ρ_D. Various lower bounds for the largest eigenvalue λ_1 of the adjacency matrix have been presented that all increase with ρ_D. The largest eigenvalue λ_1 characterizes the effect of the topology on dynamic processes on graphs. The degree-preserving rewiring algorithm is applied to a real-world network, the USA air transportation network, with the aim to make this network more robust against virus spread, given that resources, the number of flights in each airport, are constant. A general observation is that, increasing λ_1 by increasing the assortativity, relatively rapidly leads to disconnectivity, while increasing disassortativity seems to increase the algebraic connectivity μ_{N-1}, thus the topological robustness. The latter agrees with the upper bound (16) on μ_{N-1}, that indeed decreases with ρ_D.

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A Erdős-Rényi random graph

As mentioned in Section 2, we need to compute $\rho\left(D_{l^+}, D_{l^-}\right)$, where $D_{l^+} = D_i - 1$ *and* node i is connected to node j. The fact that $G_p(N)$ is connected restricts $p > p_c \sim \frac{\log N}{N}$, where p_c is the disconnectivity threshold. We first compute the joint probability $\Pr\left[D_i(N) = k, D_j(N) = m | a_{ij} = 1\right]$, where node i and node j are random nodes in $G_p(N)$. Given the existence of the direct link $a_{ij} = 1$, the direct link is counted both in D_i and in D_j such that

$$\begin{aligned}&\Pr\left[D_i(N) = k, D_j(N) = m | a_{ij} = 1\right]\\&= \Pr\left[D_i(N-1) = k-1\right]\Pr\left[D_j(N-1) = m-1\right]\end{aligned}$$

Introducing the binomial density of $\Pr\left[D_i(N) = k\right]$, we obtain

$$\begin{aligned}&\Pr\left[D_i(N) = k, D_j(N) = m | a_{ij} = 1\right]\\&= \binom{N-2}{k-1} p^{k-1}(1-p)^{N-1-k}\binom{N-2}{m-1} p^{m-1}(1-p)^{N-1-k}\end{aligned}$$

The joint expectation is

$$
\begin{aligned}
&E\left[D_i\left(N\right)D_j\left(N\right)|a_{ij}=1\right] \\
&=\sum_{k=0}^{N-1}\sum_{m=0}^{N-1} mk\Pr\left[D_i\left(N\right)=k,D_j\left(N\right)=m|a_{ij}=1\right] \\
&=\sum_{k=0}^{N-1}\left(k\binom{N-2}{k-1}p^{k-1}\left(1-p\right)^{N-1-k}\cdot\right. \\
&\left.\sum_{m=0}^{N-1} m\binom{N-2}{m-1}p^{m-1}\left(1-p\right)^{N-1-k}\right) \\
&=\left(1+(N-2)p\right)^2
\end{aligned}
$$

Next,

$$E\left[D_i\left(N\right)|a_{ij}=1\right]=1+(N-2)p$$

such that, for all N and $p>p_c$,

$$
\begin{aligned}
&\operatorname{Cov}\left[D_i\left(N\right),D_j\left(N\right)|a_{ij}=1\right] \\
&=E\left[D_i\left(N\right)D_j\left(N\right)\right]-E\left[D_i\left(N\right)\right]E\left[D_j\left(N\right)\right]=0
\end{aligned}
$$

and, hence, $\rho_D=0$: the connected Erdős-Rényi random graph $G_p\left(N\right)$ is zero-assortative.