Graph entropy, degree assortativity, and hierarchical structures in networks

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We connect several notions relating the structural and dynamical properties of a graph. Among them are the topological entropy coming from the vertex shift, which is related to the spectral radius of the graph's adjacency matrix, the Randić index, and the degree assortativity. We show that, among all connected graphs with the same degree sequence, the graph having maximum entropy is characterized by a hierarchical structure; namely, it satisfies a breadth-first search ordering with decreasing degrees (BFD ordering for short). Consequently, the maximum-entropy graph necessarily has high degree assortativity; furthermore, for such a graph the degree centrality and eigenvector centrality coincide. Moreover, the notion of assortativity is related to the general Randić index. We prove that the graph that maximizes the Randić index satisfies a BFD ordering. For trees, the converse holds as well. We also define a normalized Randić function and show that its maximum value equals the difference of Shannon entropies of two probability distributions defined on the edges and vertices of the graph based on degree correlations.

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I. INTRODUCTION

Since the beginning of the recent interest in complex networks, a major theme has been to understand the relations between various network descriptors and their connection to the network's function [1,2]. This is a daunting task since there is a large number of quantitative measures used in network studies, each one typically capturing only a particular aspect of the network. While correlations may be observed in numerical or experimental studies, rigorous relations between them may be difficult to establish or may even be nonexistent [3]. The aim of this article is to rigorously connect several network descriptors and concepts using mathematical tools.

The central notion of the paper is that of entropy, which plays a fundamental role in many areas of the physical sciences in quantifying disorder and complexity, and as such is a particularly relevant notion for studying complex systems and networks. Topological graph entropy, by its definition, is a measure of the complexity of a certain dynamical system, the so-called vertex shift, on the graph [4]. Algebraically, it can be expressed in terms of the logarithm of the spectral radius of the graph (the dominant eigenvalue of the adjacency matrix) [5,6], which in turn is related to several other types of dynamics on graphs, as we briefly mention in the next section. Therefore, it is of practical interest to characterize high- or low-entropy graphs within a suitable class. We are particularly interested in the class $\mathcal{C}_\pi$ of graphs having a given degree sequence π, motivated partly by the well-known procedure of rewiring the links in a network while keeping the vertex degrees fixed, as a means of investigating the relation between network structure and function.

Another central player of the paper, which at first sight seems unrelated to the concept of entropy, is the so-called *Randić index* R, introduced in the 1970s to study chemical compounds [7], and subsequently generalized to a family of indices R_α parametrized by a real number α (e.g., Refs. [8,9]). We will see that the topological entropy is bounded from below by $\log R_\alpha$ (up to a multiplicative constant), so that networks with a high Randić index necessarily have higher entropy. More interestingly, the Randić index, being essentially the sum of products of vertex degrees (weighted with an exponent α) over the edges, is naturally related to degree-degree correlations in the graph. We obtain that *assortative* networks, where high-degree vertices are more likely to be connected to other high-degree vertices [10], have necessarily high entropy. Stated differently, low-entropy networks are *disassortative*.

Our main contribution, however, is a much more detailed characterization of the structure of maximum-Randić as well as maximum-entropy graphs having a given degree sequence. We give a description in terms of the *breadth-first-search algorithm*, which is well known from theoretical computer science for applications like finding vertices in a connected component or the shortest path between two nodes [11]. We use a modified version taking vertex degrees into account, and say that a graph has *BFD ordering* if it satisfies a breadth-first search ordering with decreasing degrees, to be defined precisely in the paper. We prove that the graphs having the largest Randić index or the largest entropy in the class $\mathcal{C}_\pi$ satisfy a BFD ordering. Moreover, the eigenvector centrality

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measure in these extreme graphs is consistent with the degree centrality. We give a stronger result for trees, proving that the property of BFD ordering is both necessary and sufficient for a tree to have the largest Randić index or the largest entropy among all trees with a given degree sequence.

Finally, we define a *normalized Randić function* that fits better with the notion of entropy. We show that at its maximum point, the normalized Randić function equals the difference of the Shannon entropies of two natural probability measures defined on the edge and vertex sets of the graph. These results provide rigorous connections between the concepts of entropy, Randić index, degree correlations, and the graph structure.

II. TOPOLOGICAL GRAPH ENTROPY

We first recall some basic notions related to entropy and its relation to graphs, and introduce the notation. Let $G = (V, E)$ be a finite connected graph on n vertices with vertex set V and edge set E. Let $A(G) = [a_{ij}]$ denote the adjacency matrix of G, where a_{ij} equals 1 if there is an edge from vertex i to j and zero otherwise. As a simple dynamical process on the graph, consider walking along the edges. Labeling the vertices by distinct symbols from some symbol set $\mathcal{S}$, let X denote the set of all infinite symbol sequences $\{\ldots, s_{i-1}, s_i, s_{i+1}, \ldots\}$, $s_i \in \mathcal{S}$, that can be obtained by such walks, and let $\sigma : X \to X$ be the shift map that shifts each sequence to the left by one element, that is, $[\sigma(x)](i) = x(i+1)\ \forall i$ and $x \in X$. The pair (X, σ) defines a dynamical system called a *shift space* over the alphabet $\mathcal{S}$ (also called a *vertex shift*) [4]. The diversity of symbol sequences that can be produced by walks on G gives a natural measure of the complexity of the dynamics of (X, σ). To quantify, let $B_k(X)$ be the set of all blocks of length k that are present in elements of X. The *topological entropy* for the system is defined as [12]

$$H(X) = \lim_{k\to\infty} \frac{\log |B_k(X)|}{k}, \tag{1}$$

where $|\cdot|$ denotes the cardinality of a set [13]. We also write this quantity as $H(G)$, and call it the *topological entropy of the graph* G, since it arises directly from the graph structure of G.

It is well known that the walks on the graph G can be enumerated through its adjacency matrix. Indeed, the entries $[A^k]_{ij}$ of the kth power of $A(G)$ yield the number of walks of length k from vertex i to j. Thus, denoting $\mathbf{1} = (1, 1, \ldots, 1)^\top \in \mathbb{R}^n$, the quantity $N_k = \langle \mathbf{1}, A^k \mathbf{1} \rangle$, called the *Schwarz constant* of G, gives the number of walks of length k. Furthermore, since $A(G)$ has non-negative entries, Perron-Frobenius theory asserts that $A(G)$ has a non-negative dominant eigenvalue, denoted $\lambda(G)$, which equals its spectral radius, and one has [5,6]

$$\lim_{k\to\infty} (N_k)^{1/k} = \lambda(G).$$

Taking logarithms and observing that $|B_k| = N_k$ in (1), we reach the fundamental relation

$$H(G) = \log \lambda(G). \tag{2}$$

The combinatorial concept of graph entropy is related to the Shannon entropy through a variational principle, which is the analog of the Gibbs variational principle in statistical mechanics. Hence, instead of counting all possible walks on the graph without assigning any particular rules for the walk, we consider a stochastic process by assigning a probability distribution $\{p_{ij}\}$ to the outgoing edges of each vertex i. Thus, $p_{ij} \geqslant 0$ and $\sum_j p_{ij} = 1$ for all $i \in V$, and one obtains a Markov chain on n states whose state transitions are described by the stochastic matrix $P = [p_{ij}]$. Let π denote its stationary distribution, $\pi P = \pi$. The *dynamical entropy* (also called the entropy rate or the entropy production) of P is defined as [14,15]

$$h(P) = -\sum_{i=1}^{n} \pi_i \sum_{j=1}^{n} p_{ij} \log p_{ij}. \tag{3}$$

Note that the inner sum represents the classical Shannon entropy of the probability distribution $[p_{i1}, \ldots, p_{in}]$, and h is the weighted average of these entropies over the states. Now, for a given graph $G = (V, E)$ on n vertices, let M_G denote all compatible stochastic matrices P, in the sense that $p_{ij} = 0$ if $ij \notin E$. In other words, M_G represents the set of all Markov processes on n states where the possible transitions are described by the graph structure G. One can then show that [16]

$$H(G) = \sup_{P\in M_G} h(P). \tag{4}$$

Furthermore, it can be shown that the supremum is achieved by the unique stochastic matrix $P^* = [p^*_{ij}]$ defined by

$$p^*_{ij} = \frac{a_{ij} f_j}{\lambda(G) f_i}, \tag{5}$$

where $f = (f_1, \ldots, f_n)$ is the *Perron vector* of $A(G)$, that is, the unique positive eigenvector corresponding to the eigenvalue $\lambda(G)$ and satisfying $\sum_i f_i = 1$. The graph entropy is then the entropy calculated by (3) for the process P^*. Using (5) in (3) yields

$$H(G) = h(P^*) = \log \lambda(G),$$

which is the same as (2). Thus, the information-theoretic description based on the variational principles (3) and (4) is equivalent to the combinatorial definition (1) of the graph entropy. It is worth noting the important role played by the Perron vector f in characterizing the maximum-entropy process P^*. Later we will use the Perron vector to characterize the maximum-entropy graphs within the set of all graphs having the same degree sequence.

In addition to the Markov chain formulation, there are other important examples that connect graph entropy to the dynamical processes on the graph, especially when the adjacency matrix appears in the equations of motion (or their linearization). For example, in a recent discrete-time Boolean network model of genetic control [17], the stability of the steady state against small perturbations is described by the equation $\mathbf{y}(t+1) = qA\mathbf{y}(t)$, where y is the vector of perturbations and $q \in [0, 1]$ is related to the "bias" of the random output function (here assumed to be the same for each vertex). The unperturbed state is thus asymptotically stable if the dominant eigenvalue of the matrix qA is less than 1, or, by (2), $H(G) + \log q < 0$. Hence, a smaller value of entropy indicates a more robust system, in the sense that external

perturbations die down more rapidly or a wider range of values for q can be allowed without introducing instability. Similar considerations apply to population dynamics, for instance, to age-structured population models that go back to Ref. [18]. Here, the so-called *Leslie matrix A* describes the movements between age groups through births and aging, and its dominant eigenvalue λ corresponds to the asymptotic growth rate of the population. For further information on the entropic interpretation of population dynamics, the reader is referred to Refs. [16,19]. An extension of the evolutionary ideas of population dynamics to general networks is given in Ref. [15], where, using an evolutionary model based on entropy as a selective criterion, the authors give support for the hypothesis that network entropy as defined by (2) is a quantitative measure of robustness, and argue that the evolutionarily stable states of evolved networks will be characterized by extremal values of graph entropy.

We note that there are other definitions of entropy for networks used in graph theory (e.g., Refs. [20,21]) and statistical physics (e.g.. Refs. [22–26]). The definition (2) we adopt here is a natural choice due to its relation to dynamics as well as its close connection to several other graph properties, as we explore in the following sections. Motivated by the examples above, we will particularly be interested in the properties of maximum-entropy graphs.

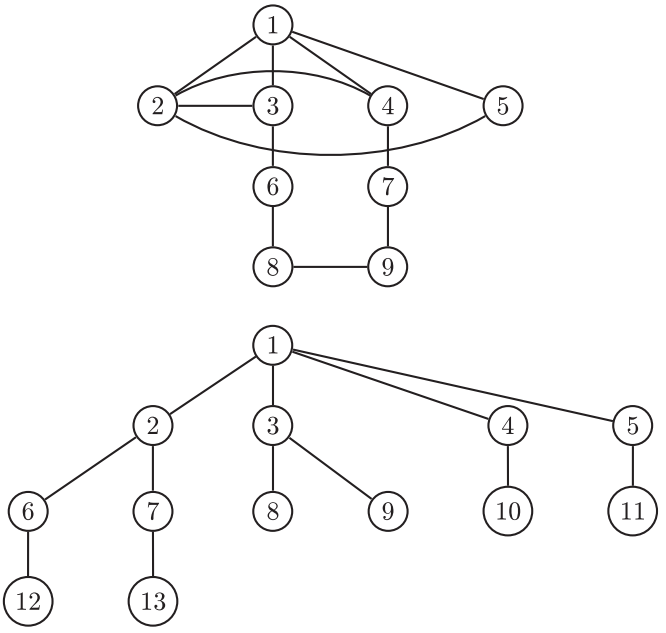

FIG. 1. Top: A BFD ordering of the degree sequence (4,4,3,3,2,2,2,2,2); Bottom: BFD ordering of the tree sequence (4,3,3,2,2,2,2,1,1,1,1,1,1).

III. ENTROPY, SPECTRAL RADIUS, AND BFD ORDERING

For the remainder of the paper we confine ourselves to simple, finite, connected, undirected graphs.

The largest eigenvalue of the adjacency matrix, also called the *spectral radius* of the graph, has several uses in network theory; for example, it has been related to the percolation threshold and the appearance of a giant component [27]. A well-known fact from graph theory is that the spectral radius is nondecreasing with respect to adding edges to a graph. This is easily understood from the entropy interpretation of the vertex shift (1), but can also be proved alternatively (e.g., Ref. [28]). Moreover, if $d_{\min}$, d_{avg}, and $d_{\max}$ denote, respectively, the smallest, average, and largest vertex degrees in a graph, then [28]

$$d_{\min} \leqslant d_{\text{avg}} \leqslant \lambda(G) \leqslant d_{\max}. \tag{6}$$

Denoting the degree of vertex v by d_v, a sequence $\pi = (d_0, \ldots, d_{n-1})$ of non-negative integers in nonincreasing order is called *degree sequence* if there exists a graph G with n vertices for which the d_i are its vertex degrees. The set of all connected graphs with degree sequence π is denoted by $\mathcal{C}_\pi$.

We introduce an ordering $\prec$ of the vertices $v_0, \ldots, v_{n-1}$ of a graph with respect to breadth-first search as follows (see Fig. 1). Select a vertex $v_0 \in G$ with the largest degree and create a sorted list of vertices beginning with v_0; append all neighbors $v_1, \ldots, v_{d_{v_0}}$ of v_0 sorted by decreasing degrees; then append all neighbors of v_1 that are not already in this list; continue recursively with $v_2, v_3, \ldots$ until all vertices of G are processed. In this way we build layers where each vertex v in layer i has distance i from root v_0. A vertex v in layer i is adjacent to some vertex w in layer $i-1$. We call the least one (in the above breadth-first search) the *parent* of v and v a child of w. Finally, this ordering $\prec$ is called *breadth-first search ordering with decreasing degrees* (BFD ordering for short) if the following hold for all vertices $v, w \in V$:

(1) If $w_1 \prec w_2$, then $v_1 \prec v_2$ for all children v_1 of w_1 and v_2 of w_2;

(2) If $v \prec u$, then $d_v \geqslant d_u$.

Thus, we begin with a largest degree on top, the vertex degrees are nonincreasing as we go down the layers, and also in each layer the vertices are sorted in nonincreasing order (Fig. 1).

We remark that for every degree sequence π, $\mathcal{C}_\pi$ has at least one graph with a BFD ordering. This can be easily seen by the well-known result of Havel and Hakimi [29,30]: A sequence of integers $d_0, d_1 \geqslant \cdots \geqslant d_n > 0, n \geqslant 2$, is a degree sequence if and only if there exists a degree sequence with $d_1 - 1, \ldots, d_{d_0+1} - 1, d_{d_0+2}, \ldots, d_n$. Here, we can choose any degree as d_0. By using the Havel-Hakimi condition, we can have BFD ordering as described above, by choosing v_0 as the vertex with the largest degree d_0 at the beginning and for further steps by choosing $d_1, \ldots, d_{d_0+1}$ in order, and so on.

With this notation we can now describe the structure of the graph having the largest entropy in a class $\mathcal{C}_\pi$. Our characterization is based on the necessary condition obtained by Bıyıkoğlu and Leydold [31] for a connected graph to have the maximum spectral radius for a given degree sequence, and the relation (2) between the spectral radius and entropy.

Theorem 1 ([31]). Let G be the graph having the largest spectral radius (and hence the largest entropy) in the class $\mathcal{C}_\pi$. Then, there exists a BFD ordering of $V(G)$ that is consistent with its Perron vector f in such a way that $f(u) > f(v)$ implies $u \prec v$ and hence $d_u \geqslant d_v$.

To gain some intuitive understanding of the graph structure implied by Theorem 1, we first note the connection to the concept of *vertex centrality*, that is, determining which vertices in the network are the more important ones [32]. Two

of the most commonly used vertex centrality measures are the *degree centrality*, which quantifies the importance of a vertex by the number of its neighbors, and *eigenvector centrality*, which orders the importance of the vertices according to the entries of the Perron vector of the adjacency matrix. Theorem 1 states that eigenvector centrality is consistent with degree centrality in maximum-entropy networks.

Furthermore, recall formula (5) for the extremal Markov process P^*, whose entropy equals the topological entropy of the graph. On an undirected graph, the process P^* maximizing information entropy has the property that

$$\frac{p^*_{uv}}{p^*_{vu}} = \left(\frac{f_v}{f_u}\right)^2,$$

where f is the Perron vector. For the maximum-entropy graph G, Theorem 1 implies that $d_v \geqslant d_u$ if $p^*_{uv} > p^*_{vu}$. Thus, the favored directions of state transitions for the process P^* are from lower- to higher-degree vertices.

The converse of Theorem 1 is in general not true, since the condition of having a BFD ordering is in general not sufficient for maximum spectral radius [31]. On the other hand, for trees the condition of BFD ordering turns out to be both necessary and sufficient, as we will see in Sec. V. In other words, there is a unique BFD-ordering tree with maximum entropy in the class of all trees having a given degree sequence.

IV. THE RANDIĆ INDEX AND DEGREE ASSORTATIVITY

Theorem 1 describes the structure of maximum-entropy graphs using the concept of BFD ordering. In this section we will show that the BFD ordering also describes the structure of graphs that are maximal with respect to another graph measure, the so-called *Randić index*. This allows us to connect the concepts of graph entropy and Randić index. Furthermore, we show that the latter is related to degree assortativity, thus bringing all these graph measures together.

The Randić index $R_\alpha(G)$ of a graph G is defined by

$$R_\alpha(G) = \sum_{vw\in E} (d_v d_w)^\alpha \tag{7}$$

for a real parameter α, where the sum is over the edges of the graph. Milan Randić [7] originally proposed the index for $\alpha = -1$ and $\alpha = -1/2$ for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. The case $\alpha = 1$ is called the *second Zagreb index*. Bollobás and Erdős generalized the index to $\alpha \in \mathbb{R}$ [8]. There are several applications of the general Randić index related to medical and pharmacological problems [9]. In the following, we investigate its relations to entropy and degree correlations.

A. Relation to Renyi and Tsallis entropies

For a probability distribution $\{p_i\}_{i=1}^n$, the Renyi entropy of order α is defined as

$$H_\alpha = \frac{1}{1-\alpha} \log\left(\sum_{i=1}^n p_i^\alpha\right)$$

for $\alpha \neq 1$ [33]. The limit $\lim_{\alpha\to 1} H_\alpha$ exists and is equal to the Shannon entropy $-\sum_i p_i \log p_i$. Consider now a probability measure on the edge set E given by

$$p_E(uv) := \frac{(d_u d_v)}{\sum_{uv\in E}(d_u d_v)} = \frac{(d_u d_v)}{R_1}. \tag{8}$$

The associated Renyi entropy can be expressed in terms of the Randić index as

$$H_\alpha = \frac{1}{1-\alpha} \log \sum_{uv\in E} \frac{(d_u d_v)^\alpha}{R_1^\alpha} = \frac{1}{1-\alpha} \log\left(\frac{R_\alpha}{R_1^\alpha}\right).$$

Similarly, the Tsallis q-entropy of the distribution $\{p_i\}_{i=1}^n$ is defined as

$$S_q = \frac{1}{q-1}\left(1 - \sum_{i=1}^n p_i^q\right)$$

for $q \neq 1$ [34]. The limit $\lim_{q\to 1} S_q$ exists and is equal to the Shannon entropy as before. For the probability distribution (8), we have

$$S_q = \frac{1}{q-1}\left(1 - \frac{R_q}{R_1^q}\right).$$

B. Relation to graph entropy

Our main aim is to relate the Randić index to topological graph entropy $\log\lambda(G)$. The next proposition shows that $\log R_\alpha$ essentially bounds $\log\lambda(G) = H(G)$ from below for a given degree sequence.

Proposition 1. For any $\alpha \in \mathbb{R}$,

$$\lambda(G) \geqslant \frac{2R_\alpha(G)}{\sum_{v\in V}(d_v)^{2\alpha}}. \tag{9}$$

Consequently, within the class $\mathcal{C}_\pi$, graphs having a large Randić index also have high topological entropy.

Proof. Consider the Rayleigh quotient on functions $f : V(G) \to \mathbb{R}$ for the largest eigenvalue:

$$\lambda(G) = \max_{f\neq 0} \frac{\langle Af, f\rangle}{\langle f, f\rangle} = \max_{f\neq 0} \frac{\sum_{v\in V} f(v) \sum_{uv\in E} f(u)}{\sum_{v\in V} f(v)^2} = \max_{f\neq 0} \frac{2\sum_{uv\in E} f(u)f(v)}{\sum_{v\in V} f(v)^2}.$$

Choosing f as $f(u) = (d_u)^\alpha$ establishes (9). The second statement of the proposition follows by noting that the denominator of (9) is fixed for a given degree sequence. ■

Remark 1. The expression (9) becomes an equality for certain graphs, so it cannot, in general, be improved further. We give two examples, namely, regular graphs and complete bipartite graphs. For a d-regular graph G, it is well known that the spectral radius is $\lambda(G) = d$. Moreover, $R_\alpha(G) = |E(G)|d^{2\alpha}$ and $\sum_{v\in V}(d_u)^{2\alpha} = d^{2\alpha}|V(G)|$, so the right-hand side of (9) becomes $2|E(G)|/|V(G)| = d$ as well. Hence, for regular graphs, (9) holds as equality for any α. The second example is complete bipartite graphs $K_{s,t}$: It is well known that $\lambda(K_{s,t}) = \sqrt{st}$ (see, e.g., Ref. [5]). One partition of $K_{s,t}$ has s vertices, each having vertex degree t, and the other partition has t vertices, each having degree s. Also, $|E(K_{s,t})| = st$. Hence, $R_\alpha(K_{s,t}) = st(ts)^\alpha = (st)^{\alpha+1}$ and $\sum_{v\in V}(d_u)^{2\alpha} = s(t^{2\alpha}) + t(s^{2\alpha}) = st(t^{2\alpha-1} + s^{2\alpha-1})$. Therefore, the right-hand side of (9) becomes $\frac{2(st)^\alpha}{t^{2\alpha-1}+s^{2\alpha-1}}$, which is equal to $\sqrt{st}$ for

$\alpha = 1/2$. Hence, for complete bipartite graphs, (9) holds as equality for $\alpha = 1/2$.

Remark 2. Note that R_0 equals the number of edges in the graph; so the right-hand side of (9), evaluated at $\alpha = 0$, is the average degree. Thus, the lower bound $\lambda(G) \geqslant d_{\text{avg}}$ in (6) follows from (9) with $\alpha = 0$. On the other hand, taking $\alpha = \frac{1}{2}$ yields the improved estimate

$$\lambda(G) \geqslant \frac{1}{|E|} \sum_{vw \in E} \sqrt{d_v d_w}.$$

C. Relation to degree assortativity and BFD ordering

Proposition 1 shows that, for a given degree sequence, graphs with high Randić index R_α also have high entropy. Thus, a natural way to seek high-entropy graphs (having a given degree sequence) is by increasing R_α. By (7), for $\alpha > 0$, the summands that contribute to R_α the most are those for which d_u and d_v are both large over an edge $uv \in E$. Hence, a high value of Randić index is expected for graphs whose high-degree vertices are connected to other high-degree vertices. Interestingly, this latter property has independently attracted attention in recent literature as a characteristic of certain real-world networks. Indeed, in social networks vertices with a high degree are often found to be adjacent to other high-degree vertices, a tendency referred to as *assortative mixing* or *assortativity*, whereas technological and biological networks typically exhibit *disassortative mixing*, where high-degree vertices are more likely to be attached to low-degree vertices [35]. Thus, the Randić indices R_α for $\alpha > 0$ act as a set of measures for the degree assortativity of networks, with α quantifying the relative weight assigned to higher degree correlations. We note that the measure denoted $s(G)$ in Ref. [36] actually corresponds to a Randić index with $\alpha = 1$. It has been shown in Refs. [37] that $s(G)$ is closely related to the assortativity measure r used in Ref. [10]. We refer the reader to Sec. 5.4 of Ref. [37] for a detailed discussion of the connection between r and $s(G)$ (and hence R_1).

Through the Randić index, we have a means of connecting degree assortativity to graph entropy using Proposition 1. Recalling that the denominator in (9) is fixed for a given degree sequence, we can state the result as follows.

Corollary 1. Among all networks having the same degree sequence, assortative networks have high entropy, or equivalently, low-entropy networks are necessarily disassortative.

A question that naturally arises is how to increase the Randić index within $\mathcal{C}_\pi$, i.e., alter the degree assortativity without changing the degree sequence. There are systematic ways of moving inside the class $\mathcal{C}_\pi$, for example, by the *edge switching* operation: Recall that, if $xy, ab \in E$ are two edges of $G = (V, E)$ and $xa, yb \notin E$, switching refers to replacing the edges xy and ab by xa and yb, respectively, thus obtaining a new graph G' with the same degree sequence; see Fig. 2. Now after such a switching operation, R_α changes by an amount ΔR_α equal to

$$(d_x d_a)^\alpha + (d_y d_b)^\alpha - (d_x d_y)^\alpha - (d_a d_b)^\alpha = \left(d_b^\alpha - d_x^\alpha\right)\left(d_y^\alpha - d_a^\alpha\right).$$

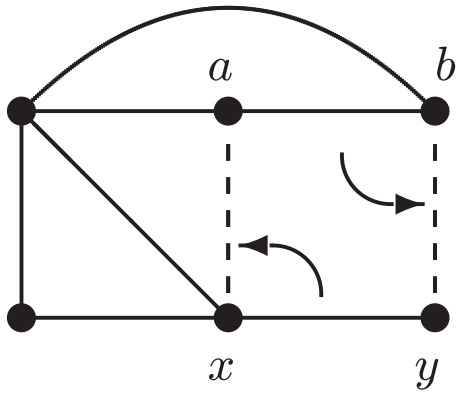

FIG. 2. An edge switching operation that increases the Randić index without changing the degree sequence. Here, the edges xy, ab are replaced by xa, yb. The reverse operation yields an example of an edge switch that decreases the Randić index.

Hence, for $\alpha > 0$, $R_\alpha(G') < R_\alpha(G)$ whenever $d_y > d_a$ and $d_x > d_b$, or by obvious symmetry, $d_y < d_a$ and $d_x < d_b$. In other words, if the new neighbors of the dissolved pair x, y have both higher or both lower degrees than the original neighbors y, x, the Randić index decreases after the switching operation. Conversely, if one vertex of the dissolved pair finds a higher-degree neighbor while the other one finds a lower-degree neighbor, as compared their original neighbors, the Randić index increases. An example is depicted in Fig. 2.

So, what does the graph having the largest Randić index for a given degree sequence look like? Our next result shows that it has a BFD-ordering structure.

Theorem 2. Let $\alpha > 0$ and let G be the graph with the largest Randić index R_α in the class $\mathcal{C}_\pi$. Then there exists a BFD ordering of $V(G)$ that is consistent with its degree sequence $d = (d_1, \ldots, d_n)$ in such a way that $d_u > d_v$ implies $u \prec v$.

Proof. Let $\alpha > 0$ and let G be the graph with the largest Randić index R_α in the class $\mathcal{C}_\pi$. Let $\pi = (d_0 \geqslant \cdots \geqslant d_{n-1})$ be the nonincreasing degree sequence of G. Create another graph G' with the same degree sequence and BFD ordering by breadth-first search, as described in Sec. III: Choose the largest degree of π as root v_0 in layer 0; append all neighbors $v_1, \ldots, v_{d(v_0)}$ of v_0 to the ordered list; these neighbors are ordered such that $u \prec v$ whenever $d_u > d_v$, or $d_u = d_v$ (in the remaining case the ordering can be arbitrary). Then, continue recursively with all degrees $d_1, d_2, \ldots$ until all degrees of π are processed. This yields the graph G' with BFD ordering. We show that either G has a BFD ordering or we get another graph G' by switching the related edges so that G has BFD ordering and $R_\alpha(G) \leqslant R_\alpha(G')$. In each recursive step we compare our graph G and G', and if the ordering is not right we switch with the proper edges, which the proof shows is always possible.

We have to show that $u \prec v$ implies $d_u \geqslant d_v$ for all $u, v \in V(G)$. Let d_v be the largest degree in π such that there exists a vertex x with $x \prec v$ but $d_x < d_v$ in G. It means that for all degrees $d > d_v$, the vertices s with $d_s > d_v$ are in the right order with respect to the ordering $\prec$. Let a and b be parents of x and v, respectively. If $a = b$, then x and v have the same parent and we can simply change their order and get a right

order for x and v. Now, we can assume that a and v are not adjacent. Firstly, observe that $d_z \leqslant d_a$ for all neighbors z of v; otherwise, the recursive BFD-ordering process must handle v for a neighbor z with $d_z > d_a$, as a *v must have come before x in the ordering* parent for v in an earlier time and it must $v \prec x$, which is a contradiction.

Secondly, v always has a neighbor p that is not adjacent to x, since $d_x < d_v$. Now we are ready to switch (replace) the edges ax and pv with edges av and xp and obtain the graph G' and $R_\alpha(G) \leqslant R_\alpha(G')$, since ΔR_α equals $d_a^\alpha d_v^\alpha + d_x^\alpha d_p^\alpha - d_a^\alpha d_x^\alpha - d_p^\alpha d_v^\alpha = (d_a^\alpha - d_p^\alpha)(d_v^\alpha - d_x^\alpha) \geqslant 0$, where p is the neighbor of v by the above observation $d_p \leqslant d_a$.

For the case $R_\alpha(G) < R_\alpha(G')$, we get a contradiction to be the largest of $R_\alpha(G)$. Observe that if $R_\alpha(G) = R_\alpha(G')$, then $d_a = d_p$ must hold. By recursive BFD-ordering construction and assumption, it holds that $a \prec p$, otherwise the process handles v as the parent of p before a and results in $v \prec x$, a contradiction. Now it follows that $v \prec x$ and we obtain a new ordering depending on p in G', and G' has more vertices in the right order than G. So we can continue the process with G'.

It remains to be shown that after replacing the edges ax and vp with av and xp, the graph G' remains connected. Since G is connected, there exists a simple path $P_{av} = (a, \ldots, t, v)$ from a to v. There are four cases to consider:

(1) If $ax \in P_{av}$ and $xt \notin E(G)$, then we set $p = t$.

(2) Else, if $ax \notin P_{av}$ and $xt \in E(G)$, then we set p to one of the neighbors of v that is not adjacent to x.

(3) Else, if $ax \in P_{av}$ and all neighbors not equal to t are adjacent to x, then t cannot be adjacent to x, and we set $p = t$.

(4) Else, $ax \in P_{av}$ and there exists a neighbor s of v, $s \neq t$, with $xs \notin E(G)$. Then, we set $p = s$.

In all cases G' remains connected. This completes the proof. ■

Remark 3. While Theorem 2 gives a necessary condition, finding a sufficient condition for the maximization of the Randić index is still an open problem. Li *et al.* [37] give a heuristic algorithm for a sufficient condition based on building a partial graph incrementally in a greedy way. However, for some degree sequences this construction can result in a disconnected graph. There do exist degree sequences, called *forcibly connected*, such that all graphs having this degree sequence are connected. A few sufficient conditions are known for a degree sequence to be forcibly connected; we mention here a result due to Bondy [38]: A degree sequence $(d_0, \ldots, d_{n-1})$ is forcibly connected if $d_i \geqslant n - i$ for every $i \geqslant d_0 + 2$. For a forcibly connected degree sequence, the heuristic algorithm of Ref. [37] computes the graph with the maximum Randić index, and by Theorem 2 this graph has a BFD ordering. However, for the special case of trees we are able to extend Theorem 2 by providing also a sufficient condition, as presented in the next section.

It has been shown that the degree distribution (or the degree sequence) of a graph does not determine the spectral gap of the graph Laplacian matrix [39]. Here we also notice that in general, by using suitable switching operations, we can get a series of graphs with the same degree sequence and different (dis)assortativity. Therefore, degree distribution and, more generally, degree sequence do not in general suffice to determine degree correlations.

V. MAXIMAL-ENTROPY AND MAXIMAL-RANDIĆ TREES

For the special case of trees, the property of BFD ordering completely characterizes the property of having maximum entropy or maximum Randić index for a given degree sequence, thereby establishing a fundamental relationship between the two concepts. In the following, the notation $\mathcal{T}_\pi$ denotes the set of all trees having degree sequence π.

Theorem 3 ([31]). A tree G with degree sequence π has the largest spectral radius in class $\mathcal{T}_\pi$ if and only if it is a BFD tree. G is then uniquely determined up to isomorphism. The BFD ordering is consistent with the Perron vector f of G, in the sense that $f(u) > f(v)$ implies $u \prec v$.

One can also compare trees having different degree sequences. To this end, let $\pi = (d_0, \ldots, d_{n-1})$ and $\pi' = (d'_0, \ldots, d'_{n-1})$ be two nonidentical sequences in nonincreasing order. We write $\pi \lhd \pi'$ if $\sum_{i=0}^{j} d_i \leqslant \sum_{i=0}^{j} d'_i$ for all $j = 0, \ldots, n-1$. Such an ordering is sometimes called *majorization*.

Theorem 4 ([31]). Let π and π' be two distinct degree sequences of trees with $\pi \lhd \pi'$, and let G and G' be trees having the largest spectral radii in classes $\mathcal{T}_\pi$ and $\mathcal{T}_{\pi'}$, respectively. Then, $\lambda(G) < \lambda(G')$.

Theorem 4 can be used to show that, among all trees with n vertices and k leaves, the largest spectral radius belongs to star-like graphs [40] with paths of almost the same lengths attached to each of its k leaves [31].

For the Randić index, we have the following counterpart to Theorem 3. It is a direct consequence of Theorem 2, and its proof is analogous to that of Theorem 3 in Ref. [31] (see also Ref. [41]).

Theorem 5. Let $\alpha > 0$. A tree G with degree sequence π has the largest Randić index R_α in class $\mathcal{T}_\pi$ if and only if it is a BFD tree. G is then uniquely determined up to an isomorphism.

VI. THE NORMALIZED RANDIĆ FUNCTION

In this section we indicate further relations between the Randić index and the concept of entropy. To this end, we also define a normalized version of the Randić index.

So far, when discussing the Randić index R_α and its relations to graph entropy and degree assortativity, the precise value of α was not specified. While most of the observations hold for any α, it is not clear whether a particular value of α has a special meaning. Even the whole set R_α, regarded as a function of $\alpha \in \mathbb{R}$, is not very enlightening—R_α is simply a monotone increasing function of α that grows unbounded as $\alpha \to \infty$. Therefore, we introduce a *normalized Randić function*:

$$\bar{R}_\alpha := \frac{\sum_{uv \in E} (d_u d_v)^\alpha}{\sum_{v \in V} (d_v)^{2\alpha}}. \tag{10}$$

The motivation for this definition is threefold. First, by Proposition 1, the spectral radius is an upper bound for $\bar{R}_\alpha$:

$$\bar{R}_\alpha \leqslant \tfrac{1}{2}\lambda(G), \quad \forall \alpha \in \mathbb{R}. \tag{11}$$

Thus, $\bar{R}_\alpha$ is a bounded continuous function of $\alpha \in \mathbb{R}$.

Second, for a k-regular graph, where each vertex has the same degree k, the Randić index is $R_\alpha = |E| k^{2\alpha}$. It is

disappointing that this quantity depends on α, namely, on how one chooses to scale the degree correlations, although the degree distribution in the graph is completely homogeneous. On the other hand, the normalized Randić for regular graphs has the constant value $\bar{R}_\alpha = |E|/|V| = \frac{1}{2}k$, independently of α.

Third, since $\bar{R}_\alpha$ is bounded, a particular value of α now naturally comes to the forefront, namely, the value $\alpha = \alpha^*$, for which $\bar{R}_\alpha$ assumes its maximum. Note that $2\bar{R}_0 = d_{\text{avg}}$; so, the maximum value $\bar{R}_{\alpha^*}$ is bounded from below by half the average degree. This and (11) give $\bar{R}_{\alpha^*}$ a place within the inequalities (6):

$$d_{\min} \leqslant d_{\text{avg}} \leqslant 2\bar{R}_{\alpha^*} \leqslant \lambda(G) \leqslant d_{\max}. \tag{12}$$

Moreover, by (2) and (11) we have a relation to graph entropy:

$$\log \bar{R}_{\alpha^*} \leqslant \log \lambda(G) - 1 = H(G) - 1.$$

We shall in fact prove a more direct relation to entropy as follows. Consider two natural probability measures on the edge set E and the vertex set V, respectively, defined by [cf. (8)]

$$\begin{aligned} p_E^\alpha(uv) &= \frac{(d_u d_v)^\alpha}{\sum_{uv\in E}(d_u d_v)^\alpha}, \\ p_V^\alpha(v) &= \frac{(d_v^2)^\alpha}{\sum_{v\in V}(d_v^2)^\alpha}. \end{aligned} \tag{13}$$

Associated with these measures are the entropy expressions

$$\begin{aligned} H_E^\alpha &= -\sum_{uv\in E} p_E^\alpha(uv)\, \log p_E^\alpha(uv), \\ H_V^\alpha &= -\sum_{v\in V} p_V^\alpha(v)\, \log p_V^\alpha(v). \end{aligned} \tag{14}$$

With this notation, we can state the following result as a fundamental relation between the entropies and the normalized Randić function.

Theorem 6. The logarithm of the normalized Randić function given by (10) satisfies

$$\frac{\partial}{\partial\alpha}\log \bar{R}_\alpha = \frac{1}{\alpha}\big(\log \bar{R}_\alpha + H_V^\alpha - H_E^\alpha\big). \tag{15}$$

Consequently, at the point $\alpha = \alpha^*$ where $\bar{R}_\alpha$ reaches its maximum,

$$\log \bar{R}_{\alpha^*} = H_E^{\alpha^*} - H_V^{\alpha^*}. \tag{16}$$

Proof. Differentiating (10) with respect to α, we have

$$\begin{aligned} \frac{\partial \bar{R}_\alpha}{\partial\alpha} &= \left[\sum_E \frac{(d_u d_v)^\alpha \log(d_u d_v)}{\sum_E (d_u d_v)^\alpha} - \sum_V \frac{d_v^{2\alpha}\log\big(d_v^2\big)}{\sum_V d_v^{2\alpha}}\right] \\ &\quad\times \frac{\sum_E (d_u d_v)^\alpha}{\log e \sum_V d_v^{2\alpha}} \\ &= \frac{1}{\alpha \log e}\left[\sum_E \frac{(d_u d_v)^\alpha \log(d_u d_v)^\alpha}{\sum_E (d_u d_v)^\alpha} - \sum_V \frac{d_v^{2\alpha}\log\big(d_v^{2\alpha}\big)}{\sum_V d_v^{2\alpha}}\right]\bar{R}_\alpha. \end{aligned}$$

By (14), the first term inside the brackets equals

$$\sum_E \frac{(d_u d_v)^\alpha}{\sum_E (d_u d_v)^\alpha}\log(d_u d_v)^\alpha = -H_E^\alpha + \log\sum_E (d_u d_v)^\alpha.$$

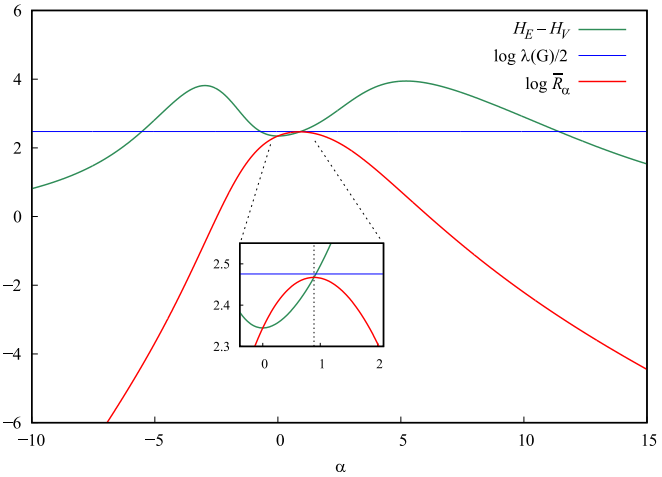

FIG. 3. Various entropic quantities calculated for a random graph G. The upper curve (green) is the difference of Shannon entropies $H_E^\alpha - H_V^\alpha$, and the lower curve (red) shows the logarithm of the normalized Randić function $\bar{R}_\alpha$, as a function of α. The horizontal line (blue) marks the value of $\log[\lambda(G)/2] = H(G) - 1$, where $H(G)$ is the topological entropy of G, which is an upper bound for $\log \bar{R}_\alpha$. The inset shows a blowup of the region where the curves meet. The maximum value of $\bar{R}_\alpha$ is attained at $\alpha^* \approx 0.89$ (vertical line in the inset).

Similarly, the second term inside the brackets equals $-H_V^\alpha + \log\sum_V d_v^{2\alpha}$. Combining,

$$\frac{\partial}{\partial\alpha}\bar{R}_\alpha = \frac{1}{\alpha\log e}\times\left(H_V^\alpha - H_E^\alpha + \log\sum_E (d_u d_v)^\alpha - \log\sum_V d_v^{2\alpha}\right)\bar{R}_\alpha,$$

which yields

$$\frac{\partial}{\partial\alpha}(\log \bar{R}_\alpha) = \log e\cdot\frac{1}{\bar{R}_\alpha}\frac{\partial}{\partial\alpha}\bar{R}_\alpha = \frac{1}{\alpha}\big(H_V^\alpha - H_E^\alpha + \log \bar{R}_\alpha\big)$$

and proves (15). Since at the maximum value of $\log \bar{R}_\alpha$ (and hence of $\bar{R}_\alpha$) the left-hand side is zero, (16) follows. ∎

We give a numerical example illustrating how various entropic concepts come together. In Fig. 3 we plot the quantities $\log \bar{R}_\alpha$ and $H_E^\alpha - H_V^\alpha$ as functions of α, calculated for an Erdős-Rényi random graph on 50 vertices where the probability of an edge between a pair of vertices is 0.2. It can be seen that at its maximum point $\alpha^* \approx 0.89$, $\log \bar{R}_\alpha$ comes very close to its theoretical upper bound $\log\lambda(G)/2$ given in (12). Moreover, at this point $\log \bar{R}_\alpha$ equals $H_E^\alpha - H_V^\alpha$.

We note that the curves $\log \bar{R}_\alpha$ and $H_E^\alpha - H_V^\alpha$ also intersect at $\alpha = 0$, in addition to α^*. This follows from the fact that the probabilities p_E^0 and p_V^0 are uniform distributions over the edge and vertex sets; so, $H_E^0 = \log|E|$, $H_V^0 = \log|V|$, and

$$\log \bar{R}_0 = \log(d_{\text{avg}}/2) = H_E^0 - H_V^0.$$

Moreover, $H_E^\alpha - H_V^\alpha$ has a local extremum at $\alpha = 0$, because the Shannon entropies H_E^α and H_V^α are maximum for uniform probability distributions, i.e., for $\alpha = 0$; so, $\frac{\partial}{\partial\alpha}(H_E^\alpha - H_V^\alpha)|_{\alpha=0} = 0$. Thus, the curves $\log \bar{R}_\alpha$ and $H_E^\alpha - H_V^\alpha$ have a

TABLE I. Various network quantities calculated on several real networks and their BFD versions: Network size $|V|$, number of edges $|E|$, average and maximum degrees, the Randić and the normalized Randić index calculated for values of $\alpha = 0.5, 1, 2$, and half the spectral radius of the graph. The minimum degree is 3 for road-chesapeake and 1 for all other networks.

Network	$\|V\|$	$\|E\|$	d_{avg}	$d_{\max}$	$R_{0.5}$	$\bar{R}_{0.5}$	R_1	$\bar{R}_1$	R_2	$\bar{R}_2$	$\lambda(G)/2$
soc-karate	34	78	4.588	17	499.50	3.2019	3640	3.0033	2.704×10^5	1.4009	3.3628
BFD					530.55	3.4010	4440	3.6634	4.625×10^5	2.3963	3.7878
soc-dolphins	62	159	5.129	12	1029.6	3.2379	7313	3.3794	4.454×10^5	3.0363	3.5968
BFD					1061.3	3.3373	8036	3.7135	5.726×10^5	3.9034	3.9385
road-chesapeake	39	170	8.718	33	1894.1	5.5710	2.347×10^4	5.2906	4.626×10^6	2.0854	5.7479
BFD					1954.5	5.7486	2.627×10^4	5.9216	6.791×10^6	3.0610	6.1670
socfb-Trinity100	2613	111 996	85.722	404	1.359×10^7	60.700	1.912×10^9	65.959	5.230×10^{13}	55.376	67.913
BFD					1.422×10^7	63.510	2.222×10^9	76.675	8.066×10^{13}	85.396	89.129
tech-routers-rf	2113	6632	6.277	109	1.155×10^5	8.7107	3.156×10^6	11.005	4.991×10^9	7.0690	13.835
BFD					1.382×10^5	10.609	5.159×10^6	18.009	1.309×10^9	18.545	22.020
web-polblogs	643	2280	7.092	165	3.970×10^4	8.7058	9.672×10^5	8.2941	1.136×10^9	1.2505	11.607
BFD					4.959×10^4	10.893	1.774×10^6	15.212	4.241×10^9	4.6687	17.122
soc-wiki-Vote	889	2914	6.556	102	4.169×10^4	7.1539	9.239×10^5	8.7440	1.250×10^9	4.5062	9.9626
BFD					4.827×10^4	8.2826	1.380×10^6	13.061	2.337×10^9	8.4245	15.231
rt-twitter-copen	761	1029	2.704	37	6147.1	2.9869	6.147×10^4	3.6352	1.725×10^7	2.3429	4.5442
BFD					7945.6	4.4142	1.240×10^5	7.4493	5.331×10^7	7.2424	8.8488
ia-infect-dublin	410	2765	13.488	50	4.951×10^4	8.9534	1.019×10^6	9.8464	5.698×10^8	8.8187	11.691
BFD					5.088×10^4	9.2000	1.120×10^6	10.817	7.709×10^8	11.932	12.417
email-univ	1133	5451	9.622	71	9.152×10^4	8.3946	1.970×10^6	9.6681	1.508×10^9	8.0208	10.374
BFD					9.995×10^4	9.1682	2.562×10^6	12.576	2.829×10^9	15.044	15.963
ca-netscience	379	914	4.823	34	6344.5	3.4707	5.563×10^4	3.7942	8.448×10^6	2.2062	5.1877
BFD					7052.4	3.8580	8.135×10^4	5.5484	2.210×10^7	5.7717	7.0869
bio-yeast	1458	1948	2.672	56	9513.5	2.4419	6.463×10^4	2.3276	7.430×10^6	0.4235	3.7675
BFD					1.281×10^4	3.7044	1.875×10^5	6.8624	9.935×10^7	5.6625	9.1127
bio-celegans	453	2025	8.940	237	4.500×10^4	11.110	1.666×10^6	10.259	8.204×10^9	2.1491	13.154
BFD					5.064×10^4	12.505	2.148×10^6	13.228	9.905×10^9	2.5947	16.687

reciprocal relationship at the two intersection points $\alpha = 0$ and $\alpha = \alpha^*$: at the former point $H_E^\alpha - H_V^\alpha$ and at the latter point the $\log \bar{R}_\alpha$ has a local extremum (inset in Fig. 3). Consequently, for $\alpha \in (0, \alpha^*)$ the various entropic quantities are related by

$$H_E^\alpha - H_V^\alpha < \log \bar{R}_\alpha < \log \lambda(G).$$

VII. NUMERICAL RESULTS ON REAL NETWORK DATA

In this section we present calculations on real network data. We have chosen 13 networks that are undirected, simple, unweighted, and connected, as we deal with such graphs in this paper. All networks are taken from The Network Repository [42,43] and are listed in Table I using the same names as in the repository. The prefixes refer to the various collections, namely, bio (biological networks), ca (collaboration networks), email (email networks), ia (interaction networks), rt (retweet networks), road (road networks), soc (social networks), socfb (Facebook networks), tech (technological networks), and web (web graphs).

For each network data and its corresponding graph, we construct a BFD-ordered graph, as explained in Sec. III. In the construction steps, in case there are several candidates with the same degree for the next vertex, we always pick one that is not yet in BFD; this guarantees that the BFD-ordered graph is connected. Since the degree sequence is not altered in the BFD construction, the network and its BFD version have identical degree information (columns 2–5 in the table). However, the Randić indices R and the spectral radii λ are significantly different. We list the Randić index R_α and the normalized Randić index $\bar{R}_\alpha$ for values of $\alpha \in \{0.5, 1, 2\}$ in columns 6–11, and calculate $\lambda(G)/2$ in the last column.

The calculations in Table I illustrate several key points of the paper. Firstly, it is seen that the Randić index R can assume very large values in large networks, whereas the normalized Randić $\bar{R}$ introduced in Sec. VI provides a more convenient magnitude. Indeed, R_α increases monotonically with α without bound, as mentioned in Sec. VI, while the normalized index $\bar{R}_\alpha$ is bounded from above. The values in the table also demonstrate the upper and lower bounds on $\bar{R}_\alpha$ given in (11) and (12). Finally, for each network, the BFD version keeps the degree sequence unchanged but markedly increases the Randić indices as well as the graph entropy $\lambda(G)$, in accordance with Theorem 2.

VIII. CONCLUSION

Entropy, as a fundamental notion for quantifying information, complexity, and disorder, is a natural concept for

complex networks. In this paper, we have established some fundamental relations between topological graph entropy, which quantifies the dynamical complexity of processes on the network structure, the Randić index from graph theory, which is related to degree assortativity, and BFD ordering from theoretical computer science, which is an algorithm for traversing graph data structures. We have introduced a normalized version of the Randić index that exhibits stronger connections to entropic quantities. These rigorous results are hoped to fuel further research in this direction for improving our understanding of complex networks.

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[1] S. Boccaletti, V. Latora, Y. Moreno, M. Chavez, and D.-U. Hwang, Complex networks: Structure and dynamics, Phys. Rep. **424**, 175 (2006).
[2] M. E. J. Newman, The structure and function of complex networks, SIAM Rev. **45**, 167 (2003).
[3] F. M. Atay, T. Bıyıkoğlu, and J. Jost, Network synchronization: Spectral versus statistical properties, Physica D **224**, 35 (2006).
[4] D. Lind and B. Marcus, *An Introduction to Symbolic Dynamics and Coding* (Cambridge University, Cambridge, 1995).
[5] D. M. Cvetković, M. Doob, and H. Sachs, *Spectra of Graphs*, 3rd ed. (Johann Ambrosius Barth, Heidelberg, 1995).
[6] M. Fujii, M. Nakamura, Y. Seo, and Y. Watatani, Graphs and Kolmogorov's complexity, Math. Jap. **44**, 113 (1996).
[7] M. Randić, On characterization of molecular branching, J. Am. Chem. Soc. **97**, 6609 (1975).
[8] B. Bollobás and P. Erdős, Graphs of extremal weights, Ars Combin. **50**, 225 (1998).
[9] X. Li and Y. Shi, A survey on the Randić index, MATCH Commun. Math. Comput. Chem. **59**, 127 (2008).
[10] M. E. J. Newman, Assortative mixing in networks, Phys. Rev. Lett. **89**, 208701 (2002).
[11] D. E. Knuth, *The Art of Computer Programming* (Addison-Wesley, Reading, 1997).
[12] S. Sternberg, *Dynamical Systems* (Dover, New York, 2010).
[13] "Log" denotes logarithm in base 2; however, the choice of the base is not important for the discussion.
[14] C. Shannon, A mathematical theory of communication, Bell Syst. Techn. J. **27**, 379 (1948).
[15] L. Demetrius and T. Manke, Robustness and network evolution–an entropic principle, Physica A **346**, 682 (2005).
[16] L. Arnold, V. M. Gundlach, and L. Demetrius, Evolutionary formalism for products of positive random matrices, Ann. Appl. Probab. **4**, 859 (1994).
[17] A. Pomerance, E. Ott, M. Girvan, and W. Losert, The effect of network topology on the stability of discrete state models of genetic control, Proc. Natl. Acad. Sci. USA **106**, 8209 (2009).
[18] P. H. Leslie, On the use of matrices in certain population mathematics, Biometrika **33**, 183 (1945).
[19] L. Demetrius, V. M. Gundlach, and G. Ochs, Complexity and demographic stability in population models, Theor. Popul Biol. **65**, 211 (2004).
[20] G. Simonyi, Perfect graphs and graph entrophy: An updated survey, in *Perfect Graphs*, edited by J. L. Ramírez Alfonsín and B. A. Reed (Wiley, Chichester, 2001).
[21] S. L. Braunstein, S. Ghosh, and S. Severini, The Laplacian of a graph as a density matrix: A basic combinatorial approach to separability of mixed states, Ann. Comb. **10**, 291 (2006).
[22] R. V. Solé and S. Valverde, Information theory of complex networks: On evolution and architectural constraints, in *Complex Networks*, edited by E. Ben-Naim, H. Frauenfelder, and Z. Toroczkai (Springer, Berlin, Heidelberg, 2004), pp. 189–207.
[23] G. Bianconi, Entropy of network ensembles, Phys. Rev. E **79**, 036114 (2009).
[24] S. Johnson, J. J. Torres, J. Marro, and M. A. Muñoz, Entropic origin of disassortativity in complex networks, Phys. Rev. Lett. **104**, 108702 (2010).
[25] K. Anand, G. Bianconi, and S. Severini, Shannon and von Neumann entropy of random networks with heterogeneous expected degree, Phys. Rev. E **83**, 036109 (2011).
[26] M. De Domenico and J. Biamonte, Spectral entropies as information-theoretic tools for complex network comparison, Phys. Rev. X **6**, 041062 (2016).
[27] B. Bollobás, C. Borgs, J. Chayes, and O. Riordan, Percolation on dense graph sequences, Ann. Probab. **38**, 150 (2010).
[28] D. Cvetković and P. Rowlinson, The largest eigenvalue of a graph: A survey, Linear Multilinear A. **28**, 3 (1990).
[29] V. Havel, Eine bemerkung zur existenz endlicher graphen, Časopis Pěst Math **80**, 477 (1955).
[30] S. L. Hakimi, On the realizability of a set of integers as degrees of the vertices of a graph, J. Ind. Appl. Math. **10**, 496 (1962).
[31] T. Bıyıkoğlu and J. Leydold, Graphs with given degree sequence and maximal spectral radius, Electron. J. Combin. **15**, R119 (2008).
[32] P. Bonacich, Factoring and weighting approaches to status scores and clique identification, J. Math. Sociol. **2**, 113 (1972).
[33] A. Rényi, On measures of entropy and information, in *Proceedings of the 4th Berkeley Symposium on Mathematical Statistics and Probability: Contributions to the Theory of Statistics* (University of California, Berkeley, 1961), Vol. 1, pp. 547–561.
[34] C. Tsallis, Possible generalization of Boltzmann-Gibbs statistics, J. Stat. Phys. **52**, 479 (1988).
[35] M. E. J. Newman, Mixing patterns in networks, Phys. Rev. E **67**, 026126 (2003).
[36] J. C. Doyle, D. L. Alderson, L. Li, S. Low, M. Roughan, S. Shalunov, R. Tanaka, and W. Willinger, The "robust yet fragile" nature of the internet, Proc. Natl. Acad. Sci. USA **102**, 14497 (2005).
[37] L. Li, D. Alderson, J. C. Doyle, and W. Willinger, Towards a theory of scale-free graphs: Definition, properties, and implications, Internet Math. **2**, 431 (2005).
[38] S. A. Choudum, On forcibly connected graphic sequences, Discrete Math. **96**, 175 (1991).

[39] F. M. Atay, T. Bıyıkoğlu, and J. Jost, Synchronization of networks with prescribed degree distributions, IEEE Trans. Circuits Syst. I **53**, 92 (2006).

[40] The kind of "star-like" graph mentioned here is obtained from a path of $n-k+1$ vertices by adding $k-1$ leaves to the first vertex.

[41] C. Delorme, O. Favaron, and D. Rautenbach, Closed formulas for the numbers of small independent sets and matchings and an extremal problem for trees, Discrete Appl. Math. **130**, 503 (2003).

[42] https://networkrepository.com/.

[43] R. A. Rossi and N. K. Ahmed, An Interactive Data Repository with Visual Analytics, SIGKDD Explor. **17**, 37 (2016).