

Article

Generalized Degree-Based Graph Entropies

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Abstract: Inspired by the generalized entropies for graphs, a class of generalized degree-based graph entropies is proposed using the known information-theoretic measures to characterize the structure of complex networks. The new entropies depend on assigning a probability distribution about the degrees to a network. In this paper, some extremal properties of the generalized degree-based graph entropies by using the degree powers are proved. Moreover, the relationships among the entropies are studied. Finally, numerical results are presented to illustrate the features of the new entropies.

Keywords: network; information theory; entropy measure; graph entropy; generalized degree-based graph entropy; degree powers

1. Introduction

Nowadays, the research of complex networks has attracted many researchers. One interesting and important problem is to study the network structure by using different graph and network measures. Meanwhile, these graph and network measures have been widely applied in many different fields, such as chemistry, biology, ecology, sociology and computer science [1–7]. From the viewpoint of information theory, the entropy of graphs was initiated to be applied by Mowshowitz [8] and Trucco [9]. Afterwards, Dehmer introduced graph entropies based on information functionals which capture structural information and studied their properties [10–12]. The graph entropies have been used as the complexity measures of networks and measures for symmetry analysis. Recently, so-called generalized graph entropies have been investigated by Dehmer and Mowshowitz [13] for better analysis and applications such as machine learning. The generalized graph entropies can characterize the topology of complex networks more effectively [14].

The degree powers are extremely considerable invariants and studied extensively in graph theory and network science, so they are commonly used as the information functionals to explore the networks [15,16]. To study more properties of graph entropies based on the degree powers, Lu et al. obtained some upper and lower bounds which have different performances to bound the graph entropies in different kinds of graphs and showed their applications in structural complexity analysis [17,18]. Inspired by Dehmer and Mowshowitz [13], we focus on the relationships between degree powers and the parametric complexity measures and then we construct generalized degree-based graph entropies by using the concept of the mentioned generalized graph entropies. The structure of this paper is as follows: In Section 2, some definitions and notations of graph theory and the graph entropies we are going to study are reviewed. In Section 3, we describe the definition of generalized degree-based graph entropies which are motivated by Dehmer and Mowshowitz [13]. In Section 4, we present some extremal properties of such entropies related to the degree powers. Moreover, we give some inequalities among the generalized degree-based graph entropies. In Section 5, numerical results of an exemplary network are shown to demonstrate the new entropies. Finally, a short summary and conclusion are drawn in the last section.

2. Preliminaries to Degree-Based Graph Entropy

A graph or network G is an ordered pair (V, E) comprising a set V of vertices together with a set E of edges. In network science, vertices are called nodes sometimes. The order of a graph means the number of vertices. The size of a graph means the number of edges. A graph of order n and size m is recorded as an (n, m) -graph. The degree of a vertex v denoted by $d(v)$ or in short d_v means the number of edges that connect to it, where an edge that connects a vertex to itself (a loop) is counted twice. The maximum and minimum degree in a graph are often denoted by $\Delta(G)$ and $\delta(G)$. If every vertex has the same degree ($\Delta(G) = \delta(G)$), then G is called a regular graph, or is called a d -regular graph with vertices of degree d . An unordered pair of vertices $\{u, v\}$ is called connected if a path leads from u to v . A connected graph is a graph in which every unordered pair of vertices is connected. Otherwise, it is called a disconnected graph. Obviously, in a connected graph, $1 \leq \delta(G) \leq \Delta(G) \leq n - 1$. A tree is a connected graph in which any two vertices are connected by exactly only one path. So tree is a connected $(n, n - 1)$ -graph. P_n is denoted a path graph characterized as a tree in which the degree of all but two vertices is 2 and the degree of the two remaining vertices is 1. S_n is denoted a star graph characterized as a tree in which the degree of all but one vertex is 1. More details can be seen in [17,18].

Next, we describe the concept of (Shannon's) entropy [19,20]. The notation "log" means the logarithm is based 2, and the notation "ln" means the logarithm is based e.

Definition 1. Let $\mathbf{p} = (p_1, p_2, \dots, p_n)$ be a probability distribution, namely, $0 \leq p_i \leq 1$ and $\sum_{i=1}^n p_i = 1$. The (Shannon's) entropy of the probability distribution is defined by

$$H(\mathbf{p}) := - \sum_{i=1}^n p_i \log p_i.$$

In the above definition, we use $0 \log 0 = 0$ for continuity of corresponding function.

Definition 2. Let $G = (V, E)$ be a graph of order n . For $v_i \in V$, we define

$$p(v_i) := \frac{f(v_i)}{\sum_{j=1}^n f(v_j)},$$

where f is a meaningful information functional. According to the information functional f , the vertices are mapped to the non-negative real numbers.

Because $\sum_{i=1}^n p(v_i) = 1$, the quantities $p(v_i)$ can be seen as probability values. Then the graph entropy of G has been defined as follows [10,12,17,18].

Definition 3. Let $G = (V, E)$ be a graph of order n and f be a meaningful information functional. The (Shannon's) graph entropy of G is defined by

$$I_f(G) := - \sum_{i=1}^n \frac{f(v_i)}{\sum_{j=1}^n f(v_j)} \log \frac{f(v_i)}{\sum_{j=1}^n f(v_j)}.$$

Definition 4. Let $G = (V, E)$ be a graph of order n . For $v_i \in V$, if $f(v_i) = d_i$, then

$$p(v_i) = \frac{d_i}{\sum_{j=1}^n d_j}.$$

Therefore, the degree-based graph entropy of G is defined as

$$I_d(G) := - \sum_{i=1}^n \frac{d_i}{\sum_{j=1}^n d_j} \log \frac{d_i}{\sum_{j=1}^n d_j}.$$

3. Generalized Degree-Based Graph Entropy

Many generalizations of entropy measure have been proposed based on the definition of Shannon's entropy [21,22]. For example, Rényi entropy [23], Daróczy's entropy [24] and quadratic entropy [25] are representative generalized entropies. In [13], Dehmer and Mowshowitz introduce a new class of generalized graph entropies that derive from the generalizations of entropy measure mentioned above and present two examples.

Definition 5. Let $G = (V, E)$ be a graph of order n . Then

$$\begin{aligned} (1). \quad I_{\alpha}^1(G) &:= \frac{1}{1-\alpha} \log \left[\sum_{i=1}^n \left(\frac{f(v_i)}{\sum_{j=1}^n f(v_j)} \right)^{\alpha} \right], \quad \alpha \neq 1; \\ (2). \quad I_{\alpha}^2(G) &:= \frac{1}{2^{1-\alpha} - 1} \left[\sum_{i=1}^n \left(\frac{f(v_i)}{\sum_{j=1}^n f(v_j)} \right)^{\alpha} - 1 \right], \quad \alpha \neq 1; \\ (3). \quad I^3(G) &:= \sum_{i=1}^n \frac{f(v_i)}{\sum_{j=1}^n f(v_j)} \left[1 - \frac{f(v_i)}{\sum_{j=1}^n f(v_j)} \right]. \end{aligned}$$

Definition 6. Let $G = (V, E)$ be a graph of order n and A its adjacency matrix. Denote by $\lambda_1, \lambda_2, \dots, \lambda_n$ the eigenvalues of G . If $f(v_i) = |\lambda_i|$, then the generalized graph entropies are as follows:

$$\begin{aligned} (1). \quad \lambda I_{\alpha}^1(G) &:= \frac{1}{1-\alpha} \log \left[\sum_{i=1}^n \left(\frac{|\lambda_i|}{\sum_{j=1}^n |\lambda_j|} \right)^{\alpha} \right], \quad \alpha \neq 1; \\ (2). \quad \lambda I_{\alpha}^2(G) &:= \frac{1}{2^{1-\alpha} - 1} \left[\sum_{i=1}^n \left(\frac{|\lambda_i|}{\sum_{j=1}^n |\lambda_j|} \right)^{\alpha} - 1 \right], \quad \alpha \neq 1; \\ (3). \quad \lambda I^3(G) &:= \sum_{i=1}^n \frac{|\lambda_i|}{\sum_{j=1}^n |\lambda_j|} \left[1 - \frac{|\lambda_i|}{\sum_{j=1}^n |\lambda_j|} \right]. \end{aligned}$$

Definition 7. Let $G = (V, E)$ be a graph of order n . Denote the collection of orbits by $S = \{V_1, V_2, \dots, V_k\}$ and their respective probabilities by $\frac{|V_1|}{n}, \frac{|V_2|}{n}, \dots, \frac{|V_k|}{n}$, where k is the number of orbits. Then another class of generalized graph entropies are derived as

$$\begin{aligned} (1). \quad {}^o I_{\alpha}^1(G) &:= \frac{1}{1-\alpha} \log \left[\sum_{i=1}^k \left(\frac{|V_i|}{n} \right)^{\alpha} \right], \quad \alpha \neq 1; \\ (2). \quad {}^o I_{\alpha}^2(G) &:= \frac{1}{2^{1-\alpha} - 1} \left[\sum_{i=1}^k \left(\frac{|V_i|}{n} \right)^{\alpha} - 1 \right], \quad \alpha \neq 1; \\ (3). \quad {}^o I^3(G) &:= \sum_{i=1}^k \frac{|V_i|}{n} \left[1 - \frac{|V_i|}{n} \right]. \end{aligned}$$

Because it is difficult to obtain the eigenvalues or the collection of orbits of graph G for a large-scale graph, and they may not meet the requirements visually, we focus on the complexity of the graphs or networks determined by the vertices themselves and the relationship between them in this paper. For a given graph G , the vertex degree is a significant graph invariant, which is related to structural properties of the graph. Most other properties of the complex network are based on the degree distribution, such as the clustering coefficient, the community structure and so on. The vertex degree in a graph or network is also intuitional and noticeable. The vertices with varying values of degree chosen as the main construction of the graph or network may decide the complexity of the graph or network. Hence, we study the generalized graph entropies based on the vertex degree and degree powers.

According to the above definitions of generalized graph entropies, let $f(v_i) = d_i$ for $v_i \in V$, then we obtain the generalized degree-based graph entropies as follows:

Definition 8.

$$(1). \quad I_{\alpha,d}^1(G) := \frac{1}{1-\alpha} \log \left[\sum_{i=1}^n \left(\frac{d_i}{\sum_{j=1}^n d_j} \right)^\alpha \right], \quad \alpha \neq 1; \quad (1)$$

$$(2). \quad I_{\alpha,d}^2(G) := \frac{1}{2^{1-\alpha} - 1} \left[\sum_{i=1}^n \left(\frac{d_i}{\sum_{j=1}^n d_j} \right)^\alpha - 1 \right], \quad \alpha \neq 1; \quad (2)$$

$$(3). \quad I_d^3(G) := \sum_{i=1}^n \frac{d_i}{\sum_{j=1}^n d_j} \left[1 - \frac{d_i}{\sum_{j=1}^n d_j} \right]. \quad (3)$$

4. Properties of the Generalized Degree-Based Graph Entropies

In this section, we will show the relationships among the stated generalized degree-based graph entropies and the degree-based graph entropy. First we will present five simple propositions which can be inferred from the Rényi entropy and [13].

Proposition 1.

$$I_{\alpha,d}^1(G) = \frac{1}{1-\alpha} \log \left[(2^{1-\alpha} - 1) I_{\alpha,d}^2(G) + 1 \right]; \quad (4)$$

$$I_{\alpha,d}^2(G) = \frac{1}{2^{1-\alpha} - 1} \left[2^{(1-\alpha) I_{\alpha,d}^1(G)} - 1 \right]; \quad (5)$$

$$I_d^3(G) = 1 - 2^{-I_{\alpha,d}^1(G)} = \frac{1}{2} I_{\alpha,d}^2(G). \quad (6)$$

Proof. Noticing that

$$\sum_{i=1}^n \left(\frac{d_i}{\sum_{j=1}^n d_j} \right)^\alpha = 2^{(1-\alpha) I_{\alpha,d}^1(G)} = (2^{1-\alpha} - 1) I_{\alpha,d}^2(G) + 1,$$

we can obtain the Equations (4) and (5). Let $\alpha = 2$, we have $\sum_{i=1}^n \left(\frac{d_i}{\sum_{j=1}^n d_j} \right)^2 = 1 - I_d^3(G)$, then the Equation (6) follows. \square

Remark 1. Proposition 1 can be seen as a special case of (12) and (16) in [13] when the value of the information functional is the degree of every vertex.

Proposition 2.

$$\lim_{\alpha \rightarrow 1} I_{\alpha,d}^1(G) = \lim_{\alpha \rightarrow 1} I_{\alpha,d}^2(G) = I_d(G) \quad (7)$$

Proof. Using l'Hôpital's rule, we can obtain the Equation (7). \square

Proposition 3. For $\alpha \in (-\infty, 1) \cup (1, +\infty)$, $I_{\alpha,d}^1(G)$ is monotonically decreasing with respect to α .

Proof. The derivative of the function $I_{\alpha,d}^1(G)$ is

$$\frac{dI_{\alpha,d}^1(G)}{d\alpha} = -\frac{1}{(1-\alpha)^2} \sum_{i=1}^n q_i \log \frac{q_i}{p_i},$$

where $q_i = \frac{d_i^\alpha}{\sum_{j=1}^n d_j^\alpha}$, $p_i = \frac{d_i}{\sum_{j=1}^n d_j}$. Then $Q = (q_1, q_2, \dots, q_n)$ and $P = (p_1, p_2, \dots, p_n)$ are also probability distributions. From the nonnegativity of Kullback-Leibler divergence, we obtain $\frac{dI_{\alpha,d}^1(G)}{d\alpha} \leq 0$. The inequality implies that $I_{\alpha,d}^1(G)$ is monotonically decreasing with respect to α . \square

Proposition 4. For $\alpha < 1$,

$$I_{\alpha,d}^1(G) \geq I_d(G); \tag{8}$$

and for $\alpha > 1$,

$$I_{\alpha,d}^1(G) \leq I_d(G); \tag{9}$$

Proof. Using Proposition 2 and Proposition 3, we can obtain the equalities above easily. \square

Remark 2. Proposition 2, Proposition 3 and Proposition 4 can be seen as the special cases of the Rényi entropy's properties.

Proposition 5.

$$I_d^3(G) < \ln 2 \cdot I_d(G). \tag{10}$$

Proof. Using the standard inequality $\ln x < x - 1$ when $x \neq 1$, we have $\ln \frac{d_i}{\sum_{j=1}^n d_j} < \frac{d_i}{\sum_{j=1}^n d_j} - 1$. Therefore,

$$\begin{aligned} I_d^3(G) &= \sum_{i=1}^n \frac{d_i}{\sum_{j=1}^n d_j} \left[1 - \frac{d_i}{\sum_{j=1}^n d_j} \right] = - \sum_{i=1}^n \frac{d_i}{\sum_{j=1}^n d_j} \left[\frac{d_i}{\sum_{j=1}^n d_j} - 1 \right] \\ &< - \sum_{i=1}^n \frac{d_i}{\sum_{j=1}^n d_j} \ln \frac{d_i}{\sum_{j=1}^n d_j} = - \ln 2 \sum_{i=1}^n \frac{d_i}{\sum_{j=1}^n d_j} \log \frac{d_i}{\sum_{j=1}^n d_j} = \ln 2 \cdot I_d(G). \end{aligned}$$

Then the inequality (10) follows. \square

Next we define the sum of the α -th degree powers as $D_\alpha := \sum_{i=1}^n d_i^\alpha$, where α is an arbitrary real number.

Theorem 1. Let $G(n, m)$ be an (n, m) -graph. Then for $\alpha \neq 1$, we have

$$(1). \quad I_{\alpha,d}^1(G) = \frac{1}{1-\alpha} \log \frac{D_\alpha}{(2m)^\alpha}; \tag{11}$$

$$(2). \quad I_{\alpha,d}^2(G) = \frac{1}{2^{1-\alpha} - 1} \left[\frac{D_\alpha}{(2m)^\alpha} - 1 \right]; \tag{12}$$

$$(3). \quad I_d^3(G) = 1 - \frac{D_2}{(2m)^2}. \tag{13}$$

Proof. By substituting $\sum_{i=1}^n d_i = 2m$ into the Equations (1)–(3), we have

$$\begin{aligned} I_{\alpha,d}^1(G) &= \frac{1}{1-\alpha} \log \left[\sum_{i=1}^n \left(\frac{d_i}{2m} \right)^\alpha \right] = \frac{1}{1-\alpha} \log \left[\sum_{i=1}^n \frac{d_i^\alpha}{(2m)^\alpha} \right] \\ &= \frac{1}{1-\alpha} \log \left[\frac{1}{(2m)^\alpha} \sum_{i=1}^n d_i^\alpha \right] = \frac{1}{1-\alpha} \log \left[\frac{D_\alpha}{(2m)^\alpha} \right]; \end{aligned}$$

$$\begin{aligned}
I_{\alpha,d}^2(G) &= \frac{1}{2^{1-\alpha} - 1} \left[\sum_{i=1}^n \left(\frac{d_i}{2m} \right)^\alpha - 1 \right] = \frac{1}{2^{1-\alpha} - 1} \left[\left(\sum_{i=1}^n \frac{d_i^\alpha}{(2m)^\alpha} \right) - 1 \right] \\
&= \frac{1}{2^{1-\alpha} - 1} \left[\frac{1}{(2m)^\alpha} \left(\sum_{i=1}^n d_i^\alpha \right) - 1 \right] = \frac{1}{2^{1-\alpha} - 1} \left[\frac{D_\alpha}{(2m)^\alpha} - 1 \right]; \\
I_d^3(G) &= \sum_{i=1}^n \frac{d_i}{2m} \left[1 - \frac{d_i}{2m} \right] = \frac{1}{(2m)^2} \sum_{i=1}^n d_i(2m - d_i) \\
&= \frac{1}{(2m)^2} \left[\left(2m \sum_{i=1}^n d_i \right) - \sum_{i=1}^n d_i^2 \right] = \frac{1}{(2m)^2} \left[(2m)^2 - D_2 \right] \\
&= 1 - \frac{D_2}{(2m)^2}.
\end{aligned}$$

So the Equations (11)–(13) hold. \square

From the above theorem, we know that the generalized degree-based graph entropies are closely related to the sum of the degree powers D_α . Obviously when $\alpha = 1$, $D_1 = \sum_{i=1}^n d_i = 2m$ presents the sum of degrees. The sum of the degree powers as an invariant is called *zeroth order general Randić index* [26–29]. For $\alpha = 2$, D_2 is also called *first Zagreb index* [30–33]. In [34], Chen et al. have reviewed D_α for different values of α and discussed the relationships with some indices such as Zagreb index, graph energies, HOMO-LUMO index, Estrada index [35–43].

Corollary 1. Let $G(n, m)$ be an (n, m) -graph. Then we have

$$1 - \frac{2m + (n-1)(n-2)}{4m(n-1)} \leq I_d^3(G) \leq 1 - \frac{1}{n}.$$

Proof. Using Cauchy-Buniakowsky-Schwarz inequality, we obtain

$$D_2 = \sum_{i=1}^n d_i^2 \geq \frac{1}{n} \left(\sum_{i=1}^n d_i \right)^2 = \frac{(2m)^2}{n}.$$

In [44] de Caen obtains the following inequality

$$D_2 = \sum_{i=1}^n d_i^2 \leq m \left(\frac{2m}{n-1} + n - 2 \right).$$

So from Equation (13), we have

$$1 - \frac{m}{(2m)^2} \left(\frac{2m}{n-1} + n - 2 \right) \leq 1 - \frac{D_2}{(2m)^2} \leq 1 - \frac{\frac{(2m)^2}{n}}{(2m)^2},$$

or equivalently,

$$1 - \frac{2m + (n-1)(n-2)}{4m(n-1)} \leq I_d^3(G) \leq 1 - \frac{1}{n}.$$

We can also find some conditions for the equalities: If G is a regular graph, then the equality $I_d^3(G) = 1 - \frac{1}{n}$ holds; If G is a tree of order n , then the equality $1 - \frac{2m+(n-1)(n-2)}{4m(n-1)}$ holds. \square

Corollary 2. Let T be a tree of order n . Then we have

$$I_d^3(S_n) \leq I_d^3(T) \leq I_d^3(P_n),$$

where S_n and P_n denote the star graph and path graph of order n , respectively.

Proof. In [45], Li and Zhao present that among all trees of order n , for $\alpha > 1$ or $\alpha < 0$, the path graph and the star graph attain the minimum and maximum value of D_α respectively; while for $0 < \alpha < 1$, the star graph and the path graph attain the minimum and maximum value of D_α respectively. Then using the Equation (13), the result of the corollary is obtained. \square

Theorem 2. When $\alpha < 1$, we have $I_{\alpha,d}^1(G) < \frac{2^{1-\alpha}-1}{(1-\alpha)\ln 2} I_{\alpha,d}^2(G)$; and when $\alpha > 1$, we have $I_{\alpha,d}^1(G) > \frac{2^{1-\alpha}-1}{(1-\alpha)\ln 2} I_{\alpha,d}^2(G)$. Especially, when $\alpha = 0$, we have $I_{\alpha,d}^1(G) = \frac{\log n}{n-1} I_{\alpha,d}^2(G)$.

Proof. First we define a new function on α on the set of real numbers \mathbb{R} as follows

$$f(\alpha) = \frac{D_\alpha}{(2m)^\alpha} = \frac{\sum_{i=1}^n d_i^\alpha}{(2m)^\alpha}.$$

Because straightforward derivative shows

$$\begin{aligned} \frac{d}{d\alpha} f(\alpha) &= \frac{1}{(2m)^\alpha} \left[\left(\sum_{i=1}^n d_i^\alpha \ln d_i \right) - \ln(2m) \left(\sum_{i=1}^n d_i^\alpha \right) \right] \\ &\leq \frac{1}{(2m)^\alpha} \left[\ln(\Delta(G)) \left(\sum_{i=1}^n d_i^\alpha \right) - \ln(2m) \left(\sum_{i=1}^n d_i^\alpha \right) \right] \\ &= \frac{\ln(\Delta(G)) - \ln(2m)}{(2m)^\alpha} \sum_{i=1}^n d_i^\alpha < 0 \text{ (by } \Delta(G) < 2m), \end{aligned}$$

we can claim that $f(\alpha)$ is a strictly decreasing function on α .

For $f(1) = 1$, we have

$$\frac{D_\alpha}{(2m)^\alpha} = \frac{\sum_{i=1}^n d_i^\alpha}{(2m)^\alpha} = \begin{cases} > 1, & \alpha < 1; \\ < 1, & \alpha > 1. \end{cases}$$

Using the standard inequality $\ln x < x - 1$ when $x \neq 1$, we find $\ln 2 \cdot \log \frac{D_\alpha}{(2m)^\alpha} < \frac{D_\alpha}{(2m)^\alpha} - 1$ when $\alpha \neq 1$.

Therefore, for $\alpha < 1$, we have

$$\frac{I_{\alpha,d}^1}{I_{\alpha,d}^2} = \frac{\frac{1}{1-\alpha} \log \frac{D_\alpha}{(2m)^\alpha}}{\frac{1}{2^{1-\alpha}-1} \left[\frac{D_\alpha}{(2m)^\alpha} - 1 \right]} < \frac{\frac{1}{(1-\alpha)\ln 2} \left[\frac{D_\alpha}{(2m)^\alpha} - 1 \right]}{\frac{1}{2^{1-\alpha}-1} \left[\frac{D_\alpha}{(2m)^\alpha} - 1 \right]} = \frac{2^{1-\alpha} - 1}{(1-\alpha)\ln 2}.$$

For $\alpha > 1$, we have

$$\frac{I_{\alpha,d}^1}{I_{\alpha,d}^2} = \frac{\frac{1}{1-\alpha} \log \frac{D_\alpha}{(2m)^\alpha}}{\frac{1}{2^{1-\alpha}-1} \left[\frac{D_\alpha}{(2m)^\alpha} - 1 \right]} > \frac{\frac{1}{(1-\alpha)\ln 2} \left[\frac{D_\alpha}{(2m)^\alpha} - 1 \right]}{\frac{1}{2^{1-\alpha}-1} \left[\frac{D_\alpha}{(2m)^\alpha} - 1 \right]} = \frac{2^{1-\alpha} - 1}{(1-\alpha)\ln 2}.$$

Especially, when $\alpha = 0$, $I_{\alpha,d}^1 = \log n$ and $I_{\alpha,d}^2 = n - 1$. So $I_{\alpha,d}^1(G) = \frac{\log n}{n-1} I_{\alpha,d}^2(G)$ holds in this case. \square

Corollary 3. When $0 \leq \alpha < 1$, we have $I_{\alpha,d}^1(G) < \frac{1}{\ln 2} I_{\alpha,d}^2(G)$.

Proof. First we define a new function on α on the set of real numbers \mathbb{R} as follows

$$g(\alpha) = 2^{1-\alpha} - 1 - (1-\alpha).$$

Because the second order derivative shows

$$\frac{d^2}{d\alpha^2}g(\alpha) = 2^{1-\alpha}(\ln 2)^2 > 0,$$

we can claim that $g(\alpha)$ is a convex function on α . Since $g(0) = g(1) = 0$, we find $2^{1-\alpha} - 1 \leq 1 - \alpha$ for $0 \leq \alpha < 1$, or equivalently $0 < \frac{2^{1-\alpha}-1}{1-\alpha} \leq 1$ for $0 \leq \alpha < 1$. Using Theorem 2, the inequality $I_{\alpha,d}^1(G) < \frac{1}{\ln 2} I_{\alpha,d}^2(G)$ holds. \square

Theorem 3. When $\alpha < 1$ and $1 < \alpha < 2$, we have $I_d^3(G) > (1 - 2^{1-\alpha})I_{\alpha,d}^2(G)$; when $\alpha > 2$, we have $I_d^3(G) < (1 - 2^{1-\alpha})I_{\alpha,d}^2(G)$; and when $\alpha = 2$, we have $I_d^3(G) = (1 - 2^{1-\alpha})I_{\alpha,d}^2(G) = \frac{1}{2}I_{\alpha,d}^2(G)$.

Proof. First we have

$$\begin{aligned} I_{\alpha,d}^2(G) - I_d^3(G) &= \frac{1}{2^{1-\alpha} - 1} \left[\frac{D_\alpha}{(2m)^\alpha} - 1 \right] - \left[1 - \frac{D_2}{(2m)^2} \right] \\ &= \frac{1}{1 - 2^{1-\alpha}} \left[1 - \frac{D_\alpha}{(2m)^\alpha} \right] - \left[1 - \frac{D_2}{(2m)^2} \right], \end{aligned}$$

and $f(\alpha) = \frac{D_\alpha}{(2m)^\alpha}$ is a strictly decreasing function on α .

Therefore, for $\alpha < 1$, $f(\alpha) > f(2)$ and $\frac{1}{1-2^{1-\alpha}} < 0$ are obtained. Then we have

$$\begin{aligned} I_{\alpha,d}^2(G) - I_d^3(G) &> \frac{1}{1 - 2^{1-\alpha}} \left[1 - \frac{D_2}{(2m)^2} \right] - \left[1 - \frac{D_2}{(2m)^2} \right] \\ &= \left(\frac{1}{1 - 2^{1-\alpha}} - 1 \right) \left[1 - \frac{D_2}{(2m)^2} \right] = \left(\frac{1}{1 - 2^{1-\alpha}} - 1 \right) I_d^3(G) \end{aligned}$$

This implies $I_d^3(G) > (1 - 2^{1-\alpha})I_{\alpha,d}^2(G)$.

For $1 < \alpha < 2$, $f(\alpha) > f(2)$ and $\frac{1}{1-2^{1-\alpha}} > 0$ are obtained. Then we have

$$\begin{aligned} I_{\alpha,d}^2(G) - I_d^3(G) &< \frac{1}{1 - 2^{1-\alpha}} \left[1 - \frac{D_2}{(2m)^2} \right] - \left[1 - \frac{D_2}{(2m)^2} \right] \\ &= \left(\frac{1}{1 - 2^{1-\alpha}} - 1 \right) \left[1 - \frac{D_2}{(2m)^2} \right] = \left(\frac{1}{1 - 2^{1-\alpha}} - 1 \right) I_d^3(G) \end{aligned}$$

This implies $I_d^3(G) > (1 - 2^{1-\alpha})I_{\alpha,d}^2(G)$.

For $\alpha = 2$, using (6) we have $I_d^3(G) = (1 - 2^{1-\alpha})I_{\alpha,d}^2(G) = \frac{1}{2}I_{\alpha,d}^2(G)$.

For $\alpha > 2$, $f(\alpha) < f(2)$ and $\frac{1}{1-2^{1-\alpha}} > 0$ are obtained. Then we have

$$\begin{aligned} I_{\alpha,d}^2(G) - I_d^3(G) &> \frac{1}{1 - 2^{1-\alpha}} \left[1 - \frac{D_2}{(2m)^2} \right] - \left[1 - \frac{D_2}{(2m)^2} \right] \\ &= \left(\frac{1}{1 - 2^{1-\alpha}} - 1 \right) \left[1 - \frac{D_2}{(2m)^2} \right] = \left(\frac{1}{1 - 2^{1-\alpha}} - 1 \right) I_d^3(G) \end{aligned}$$

This implies $I_d^3(G) < (1 - 2^{1-\alpha})I_{\alpha,d}^2(G)$. Thus we complete the proof. \square

Corollary 4. When $\alpha \geq 2$, we have $I_\alpha^3(G) < I_{\alpha,d}^2(G)$.

Proof. For $1 - 2^{1-\alpha} < 1$, we have the result by using Theorem 3. \square

Theorem 4. When $\alpha < 1$, we have $I_{\alpha,d}^1(G) > \frac{1}{\ln 2} \cdot I_d^3(G)$; when $1 < \alpha < 2$, we have $I_{\alpha,d}^1(G) < \frac{1}{(\alpha-1)\ln 2} \cdot \frac{I_d^3(G)}{1-I_d^3(G)}$; and when $\alpha \geq 2$, we have $I_{\alpha,d}^1(G) > \frac{1}{(\alpha-1)\ln 2} I_d^3(G)$.

Proof. For $\alpha < 1$, using (8) and (10) we have $I_{\alpha,d}^1(G) > \frac{1}{\ln 2} \cdot I_d^3(G)$.

For $1 < \alpha < 2$, $f(\alpha) > f(2)$ and $\frac{1}{\alpha-1} > 0$ are obtained. Then we have

$$\frac{I_{\alpha,d}^1(G)}{I_d^3(G)} = \frac{\frac{1}{1-\alpha} \log \frac{D_\alpha}{(2m)^\alpha}}{1 - \frac{D_2}{(2m)^2}} < \frac{\frac{1}{1-\alpha} \log \frac{D_2}{(2m)^2}}{1 - \frac{D_2}{(2m)^2}} = \frac{1}{(\alpha - 1) \ln 2} \cdot \frac{\ln \frac{(2m)^2}{D_2}}{1 - \frac{D_2}{(2m)^2}}$$

Using the standard inequality $\ln x < x - 1$ when $x \neq 1$, we find $\ln \frac{(2m)^2}{D_2} < \frac{(2m)^2}{D_2} - 1$. So

$$\frac{I_{\alpha,d}^1(G)}{I_d^3(G)} < \frac{1}{(\alpha - 1) \ln 2} \cdot \frac{\frac{(2m)^2}{D_2} - 1}{1 - \frac{D_2}{(2m)^2}} = \frac{1}{(\alpha - 1) \ln 2} \cdot \frac{1}{\frac{D_2}{(2m)^2}} = \frac{1}{(\alpha - 1) \ln 2} \cdot \frac{1}{1 - I_d^3(G)}$$

This implies $I_{\alpha,d}^1(G) < \frac{1}{(\alpha-1)\ln 2} \cdot \frac{I_d^3(G)}{1-I_d^3(G)}$.

For $\alpha \geq 2$, using Theorem 2 and Theorem 3 we have $I_{\alpha,d}^1(G) > \frac{2^{1-\alpha}-1}{(1-\alpha)\ln 2} I_{\alpha,d}^2(G)$ and $I_d^3(G) \leq (1 - 2^{1-\alpha}) I_{\alpha,d}^2(G)$. This implies $I_{\alpha,d}^1(G) > \frac{1}{(\alpha-1)\ln 2} I_d^3(G)$. Thus we complete the proof. \square

5. Numerical Results

In order to illuminate the principle of generalized degree-based graph entropies, we show a network in Figure 1 as an example.

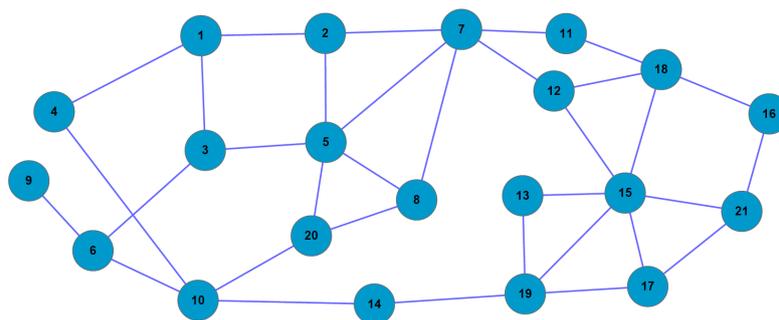


Figure 1. A simple network for example.

The degree of each node of the example network is shown in Table 1.

Table 1. The degree of each node of the example network.

node number	1	2	3	4	5	6	7	8	9	10	11
degree	3	3	3	2	5	3	5	3	1	4	2
node number	12	13	14	15	16	17	18	19	20	21	
degree	3	2	2	6	2	3	4	4	3	3	

We can easily calculate $I_d^3(G) = 0.946$. The details of $I_{\alpha,d}^1(G)$ and $I_{\alpha,d}^2(G)$ with different α are shown in Table 2.

Table 2. The generalized degree-based graph entropies $I_{\alpha,d}^1(G)$ and $I_{\alpha,d}^2(G)$ of the example network.

The Value of α	-1.0	-0.5	0.0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0
$I_{\alpha,d}^1(G)$	4.505	4.447	4.392	4.342	4.294	4.249	4.206	4.165	4.127	4.090	4.056
$I_{\alpha,d}^2(G)$	171.633	55.146	20.000	8.457	4.294	2.631	1.892	1.527	1.329	1.214	1.143

In Table 2 that the value of α is equal to 1.0 means $\alpha \rightarrow 1$. Then $I_{\alpha,d}^1(G)$ and $I_{\alpha,d}^2(G)$ are degenerated to the degree-based graph entropy $I_d(G) = 4.294$.

It is clear that following the increase of the value of α , the values of the generalized degree-based graph entropies $I_{\alpha,d}^1(G)$ and $I_{\alpha,d}^2(G)$ of the complex network are decrease. Based on the concept of the entropy, the bigger the value of the entropy is, the more complex of the network is. From the definitions of $I_{\alpha,d}^1(G)$ and $I_{\alpha,d}^2(G)$, the value of the entropic index α can be used to change the construction of the entropies. In other words, the value of α represents the relationship among the nodes in the complex network. Combined with the complex network, the influence of each node's degree on the entropies is changed by the value of α . The relationship between the value of α and the entropies of the complex network is shown as follows:

- (1) When $\alpha < 1$, the nodes with small value of degree play an important part in the construction of $I_{\alpha,d}^1(G)$ and $I_{\alpha,d}^2(G)$, or they are chosen as the main construction of the complex networks. Especially when the value of $\alpha = 0$, each node has the same influence on the whole network from the entropic point of view.
- (2) When $\alpha \rightarrow 1$, the influence of each node on the network is based on the value of degree for each node. The generalized degree-based graph entropies $I_{\alpha,d}^1(G)$ and $I_{\alpha,d}^2(G)$ are degenerated to the degree-based graph entropy $I_d(G)$. So the structure property determined by the node's degree decides the complexity of the complex network.
- (3) When $\alpha > 1$, the nodes with big value of degree play an important part in the construction of $I_{\alpha,d}^1(G)$ and $I_{\alpha,d}^2(G)$, or they are chosen as the main construction of the complex networks. The values of the entropies tend to stabilization. The complex network is tended to orderly.

To sum up, according to the definition of the generalized degree-based graph entropies of the complex network, the value of the entropic index α is used to describe the different relationship among the nodes. When the value of α is smaller than 1, the nodes with small value of degree are more important than the nodes with big value of degree. The edges among those nodes with small value of degree become the main part of the complex network. As these nodes with small value of degree are the majority in the complex network, the whole network has greater complexity. When the value of α is equal to 0, the nodes in the network are equal to each other in terms of influence. When the value of α tends to 1, $I_{\alpha,d}^1(G)$ and $I_{\alpha,d}^2(G)$ are degenerated to $I_d(G)$, the level of complexity for the complex network is decided by the structure property. In other words, the complexity of the complex network is decided by the degree sequence and degree distribution. When the value of α is trended to ∞ , the construction of the complex network is decided by the node which has a biggest value of degree, the values of $I_{\alpha,d}^1(G)$ and $I_{\alpha,d}^2(G)$ decrease to stable values, and the complex network is more orderly. The complexity of the complex network is not only decided by the structure of the complex network, but also influenced by the kind of the relationship between each node.

From Figure 2, we can see the plotted values of the generalized degree-based graph entropies $I_{\alpha,d}^1(G)$, $I_{\alpha,d}^2(G)$ and $I_d^3(G)$ relative to α ($I_{\alpha,d}^1(G)$, $I_{\alpha,d}^2(G)$ with a pole at $\alpha = 1$). The numerical results can be interpreted as follows: First we observe that the value of $I_{\alpha,d}^1(G)$ is less than that of $I_{\alpha,d}^2(G)$ for $\alpha < 1$, while the value of $I_{\alpha,d}^1(G)$ is larger than that of $I_{\alpha,d}^2(G)$ for $\alpha > 1$. Next, for $I_{\alpha,d}^1(G)$, $I_{\alpha,d}^2(G)$ and $I_d^3(G)$, we can have the values of $I_{\alpha,d}^1(G)$ and $I_{\alpha,d}^2(G)$ is always larger than that of $I_d^3(G)$. Actually, using l'Hôpital's rule we have that the value of $I_{\alpha,d}^1(G)$ tends to 3.459 and the value of $I_{\alpha,d}^2(G)$ tends to 1 when α tends to $+\infty$. At last, all the curves verify the inequalities in the Section 4.

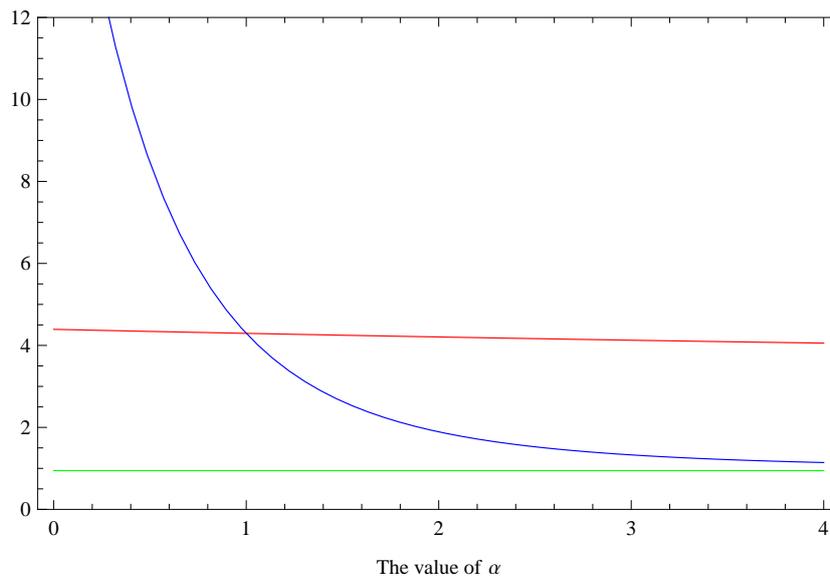


Figure 2. $I_{\alpha,d}^1(G)$ (red), $I_{\alpha,d}^2(G)$ (blue) and $I_d^3(G)$ (green) versus α . ($I_{\alpha,d}^1(G)$, $I_{\alpha,d}^2(G)$ with a pole at $\alpha = 1$).

In addition, generalized graph entropy measures with parameters have been presented to be useful in studying the complexity associated with machine learning. For example, Dehmer et al. have described that the generalized graph entropies can be applied to the graph classification and clustering cases in machine learning. The applications involve optimizing particular parameters associated with graphs or networks in given sets [4,46]. So by applying supervised machine learning methods, the generalized degree-based entropies can be used for classifying the chemical structures, developing methods for characterizing predictive models according to optimal values of relevant parameters in bioinformatics, systems biology, and drug design.

6. Summary and Conclusions

In this paper, we studied the generalized degree-based graph entropies, which are inspired by Dehmer and Mowshowitz in [13] and derived from the Rényi entropy [23], Daróczy's entropy [24] and quadratic entropy [25]. We studied the relationships between the sum of the degree powers and the new entropies. Then we examined the extremal values of the above stated entropies in terms of the sum of the degree powers. We also proved some inequalities between these generalized degree-based graph entropies. Finally, we obtained numerical values for an exemplary complex network for each of the entropies, and concluded that their parameters can influence which kind of nodes contribute to the main part of the network in terms of graph entropy theory. The generalized degree-based graph entropies expand the description methods of the structural complexity of the complex networks. They would play bigger roles in describing structural symmetry and asymmetry in real networks in the future.

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