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Article

Entropy of Weighted Graphs with Randić Weights

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Abstract: Shannon entropies for networks have been widely introduced. However, entropies for weighted graphs have been little investigated. Inspired by the work due to Eagle *et al.*, we introduce the concept of graph entropy for special weighted graphs. Furthermore, we prove extremal properties by using elementary methods of classes of weighted graphs, and in particular, the one due to Bollobás and Erdös, which is also called the Randić weight. As a result, we derived statements on dendrimers that have been proven useful for applications. Finally, some open problems are presented.

Keywords: Shannon's entropy; graph entropy; weighted graphs; extremal value; Randić weight

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1. Introduction

The study of entropy measures for exploring network-based systems emerged in the late fifties based on the seminal work due to Shannon [1]. Rashevsky is the first who introduced the so-called structural information content based on partitions of vertex orbits [2]. Mowshowitz used the the same measure and proved some properties for graph operations (sum, join, *etc.*) [3–6]. Moreover, Rashevsky used the concept of graph entropy to measure the structural complexity of graphs. Here, the complexity of a graph is based on the well-known Shannon's entropy. Mowshowitz [3] introduced the entropy of a graph as an information-theoretic quantity, and he interpreted it as the structural information content of a graph. Mowshowitz [3] later studied mathematical properties of graph entropies measures thoroughly and also discussed special applications thereof. Graph entropy measures have been used in various disciplines, for example for characterizing graph patterns in biology, chemistry and computer science; see [7–14]. Thus, it is not surprising at all to realize that the term "graph entropy" has been defined in various ways. Another classical example is Körner's entropy [15], introduced from an information theory-specific point of view.

Several graph invariants have been used for developing graph entropy measures, such as the number of vertices, the vertex degree sequences, extended degree sequences (*i.e.*, the second neighbor, third neighbor, *etc.*), eigenvalues and connectivity information; see, [16–21]. Distance-based graph entropies [17,21] are also studied, which are related to the average distance and various Wiener indices [22–32]. The properties of graph entropies that are based on information functionals by using degree powers of graphs have been explored, too; see [13,33,34]. The degree power is one of the most important graph invariants and well studied in graph theory; its also related to the Zagreb index [35–41] and the zeroth-order Randić index [42–44]. To study results on the properties of degree powers and Randić indices in depth, we refer to [45,46].

In order to investigate the influence of the structure of social relations between individuals of a community's economic development, Eagle *et al.* [47] developed two new metrics, social diversity and spatial diversity, to capture the social and spatial diversity of communication ties within a social network of each individual, by using the entropy for vertices. Following this, we introduce the concept of graph entropy for weighted graphs. We mention that Dehmer *et al.* [48] already tackled the problem of defining the entropy of weighted chemical graphs by using special information functionals. Therefore, this paper extends the work done in [48] considerably. Another contribution of this paper relates to the study of extremal values of weighted graphs. We examined the extremal properties of this entropy when using special graph classes. Here, we use the class of weighted graphs due to Bollobás and Erdös. Finally, some open problems are presented.

2. Preliminaries

In this paper, "log" denotes the logarithm based on two entirely.

In [47], the authors used the following node entropy. For a given graph G and vertex v_i, let d_i be the degree of v_i. For an edge v_iv_j, one defines:

$$p_{ij} = \frac{w(v_i v_j)}{\sum_{j=1}^{d_i} w(v_i v_j)}, \tag{1}$$

where $w(v_i v_j)$ is the weight (or volume) of the edge $v_i v_j$ and $w(v_i v_j) > 0$. The node entropy has been defined by:

$$H(v_i) = -\sum_{j=1}^{d_i} p_{ij} \log(p_{ij}). \tag{2}$$

Motivated by this method, we introduce the definition of the entropy of edge-weighted graphs, which also can be interpreted as multiple graphs. For an edge-weighted graph, $G = (V, E, w)$, where V, E and w denote the vertex set, the edge set and the edge weight (sometimes, also called the cost) of G, respectively. In this paper, we always assume that the edge weight is positive.

Definition 1. *For an edge weighted graph $G = (V, E, w)$, the entropy of G is defined by:*

$$I(G, w) = -\sum_{uv \in E} p_{uv} \log(p_{uv}), \tag{3}$$

where $p_{uv} = \frac{w(uv)}{\sum\limits_{uv \in E} w(uv)}$.

The above definition of the entropy for edge-weighted graphs is based on the probability function (1), which is used in [47]. In this sense, Definition 1 is a general case of that used by Eagle *et al.* For any edge weight w, Theorem 1 provides the extremal values of $I(G, w)$ for graphs with n vertices. However, if we want to go further to investigate the extremal values of $I(G, w)$, then we need to specify an edge weight function rather than the general case. After careful consideration, we would like to choose the Randić weight, which is well studied; for more details, see Section 3.

In the following, we assume all to be edge weighted connected graphs. Let K_n, P_n and S_n be the complete graph, the path graph and the star graph with n vertices, respectively. A tree is called a subdivided star if it is obtained from a star by subdividing each edge of the star exactly once, and at most one edge is subdivided twice. The double star with n vertices, denoted by $S_{p,q}$, is the tree obtained by connecting two centers of two stars S_p and S_q, where $p + q = n$. The balanced complete bipartite graph is a complete bipartite graph, such that the numbers of vertices in the two parts are equal or have a difference of one. The balanced complete multipartite graph is a complete multipartite graph, such that the number of vertices in any two parts are equal or have a difference of one, which is also called the Turán graph.

3. Extremal Properties of $I(G, w)$

The trivial case is that $w(e) = c > 0$ for each edge e, where c is a constant.

Theorem 1. *Let $G = (V, E, w)$ be a graph with n vertices. If $w(e) = c$ for each edge e, where $c > 0$ is a constant, then we obtain:*

$$\log(n-1) \leq I(G, w) \leq \log\left(\frac{n(n-1)}{2}\right).$$

The left equality holds if and only if G is a tree, and the right equality holds if and only if G is the complete graph.

Proof. Suppose $m = |E|$. Since $w(e) = c$ for each edge e, then we get:

$$I(G, w) = -\sum_{e \in E} \frac{1}{m} \log \frac{1}{m} = \sum_{e \in E} \frac{\log m}{m} = \log m.$$

Since G is connected, we have $n - 1 \leq m \leq \binom{n}{2}$. The result is proven. $\square$

In 1975, the chemist, Milan Randić [49], proposed a topological index by describing its interpretation as the "branching index". It has been proven useful for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. This index is nowadays called the Randić index. Randić noticed that there is a good correlation between this index and several physico-chemical properties of alkanes; for instance boiling points, chromatographic retention times, enthalpies of formation, parameters of the Antoine equation for vapor pressure, surface areas, *etc*. Later, in 1998, two famous mathematicians, Bollobás and Erdös [50], generalized this index by replacing $-1/2$ by any real number α, which is called the general Randić index. In fact, the Randić index became the most popular and most frequently-employed structure descriptor, used in numerous QSPRand QSARstudies. To study chemical applications and mathematical results of the Randić index in depth, we refer to [44,49,51].

For an edge $e = uv$ and any real number α, one defines $w(e) = (d(u)d(v))^\alpha$, where $d(u)$ denotes the degree of u. Then, the general Randić index [44,52,53] is defined as:

$$R_\alpha(G) = \sum_{uv \in E} (d(u)d(v))^\alpha. \tag{4}$$

When $\alpha = -\frac{1}{2}$, Equation (4) is just the well-known Randić index [49]. When $\alpha = 1$, Equation (4) is the second Zagreb index [54–57]. The case of $\alpha = -1$ has been also investigated [58].

Now, we list some basic extremal results on $R_\alpha(G)$ for $\alpha < 0$ that are used in this paper.

Lemma 1 ([44]). *(i) Let G be a graph with n vertices and no isolated vertices. For $\alpha \in (-1/2, 0)$, the maximum value of R_α is $\frac{n(n-1)^{1+2\alpha}}{2}$, and the minimum value is $\min\{(n-1)^{1+\alpha}, \frac{n}{2}(\text{even } n), \frac{n-3}{2} + 2^{1+\alpha}(\text{odd } n)\}$; for $\alpha \in (-\infty, -1)$, the maximum value of R_α is $\frac{n}{2}$ (even n) or $\frac{n-3}{2} + 2^{1+\alpha}$ (odd n), and the minimum value is $\frac{n(n-1)^{1+2\alpha}}{2}$.*
(ii) Among all trees with n vertices, the star graph S_n attains the minimum value of R_α for $\alpha < 0$ and $R_\alpha(S_n) = (n-1)^{\alpha+1}$; the path graph P_n attains the maximum value of R_α for $\alpha \in [-1/2, 0]$ and $R_\alpha(P_n) = 2^{\alpha+1} + (n-3)4^\alpha$; the subdivided star attains the maximum value of R_α for $\alpha \in [-\infty, -2]$ when $n \geq 7$, and the R_α-value of the subdivided star is $\frac{n-1}{2}((n-1)^\alpha + 2^\alpha)$ (odd n) or $\frac{n-2}{2}((n-2)^\alpha + 2^\alpha) + 4^\alpha$ (even n).

Let G be a graph with n vertices. The Laplacian matrix of G is $L(G) = D(G) - A(G)$, where $A(G)$ and $D(G) = diag(d_1, d_2, \ldots, d_n)$ denote the adjacency matrix of G and the diagonal matrix of vertex degrees, respectively. Let $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G) = 0$ be the eigenvalues of $L(G)$, which are also called Laplacian eigenvalues of G. In [59], the authors proved the following result.

Lemma 2 ([59]). *Let G be a simple connected graph with n vertices. Then:*

$$\frac{1}{2}\sum_{i=1}^{n} d_i^{2\alpha+1} - \frac{k}{2}\lambda_1(G) \leq R_\alpha(G) \leq \frac{1}{2}\sum_{i=1}^{n} d_i^{2\alpha+1} - \frac{k}{2}\lambda_{n-1}(G),$$

where $k = \sum_{i=1}^{n} d_i^{2\alpha} - \frac{1}{n}(\sum_{i=1}^{n} d_i^{\alpha})^2$.

Let $I(G,\alpha)$ be the entropy $I(G,w)$ based on the above stated weight, *i.e.*,

$$I(G,\alpha) = -\sum_{uv\in E} \frac{(d(u)d(v))^\alpha}{\sum_{uv\in E}(d(u)d(v))^\alpha} \log\left(\frac{(d(u)d(v))^\alpha}{\sum_{uv\in E}(d(u)d(v))^\alpha}\right).$$

The above equality can also be expressed as:

$$I(G,\alpha) = \log(R_\alpha(G)) - \frac{\alpha}{R_\alpha(G)}\sum_{uv\in E}(d(u)d(v))^\alpha \log(d(u)d(v)).$$

Now, we can establish inequalities between $I(G,\alpha)$ and R_α.

Theorem 2. *Let G be a connected graphs with n vertices. For $\alpha < 0$, we have:*

$$\log(R') - \alpha \leq I(G,\alpha) \leq \log(R) - 2\alpha\log(n-1),$$

where $R' = \min R_\alpha(G)$ and $R = \max R_\alpha(G)$.

Proof. Since $\alpha < 0$, we have:

$$I(G,\alpha) \leq \log(R) - \frac{\alpha}{R}\sum_{uv\in E}(d(u)d(v))^\alpha \log((n-1)^2) = \log(R) - 2\alpha\log(n-1)$$

and

$$I(G,\alpha) \geq \log(R') - \frac{\alpha}{R'}\sum_{uv\in E}(d(u)d(v))^\alpha \log(2) = \log(R') - \alpha.$$

The proof is completed. □

From the above stated theorem representing an upper or a lower bound of R_α for $\alpha < 0$, we can obtain an upper bound or a lower bound of $I(G,\alpha)$. As an example, we can get some bounds of R_α from Lemmas 1 and 2.

Corollary 1. *(i) Let G be a graph with n vertices and no isolated vertices. For $\alpha \in (-1/2, 0)$, we have:*

$$\log\left(\min\{(n-1)^{1+\alpha}, \frac{n}{2}(even\, n), \frac{n-3}{2} + 2^{1+\alpha}(odd\, n)\}\right) - \alpha \leq I(G,\alpha) \leq \log\left(n(n-1)\right) - 1;$$

for $\alpha \in (-\infty, -1)$, when n is even, we have:

$$\log\left(n(n-1)^{1+2\alpha}\right) - \alpha - 1 \leq I(G,\alpha) \leq \log\left(n\right) - 2\alpha\log(n-1) - 1,$$

when n is odd, we have:

$$\log\left(n(n-1)^{1+2\alpha}\right) - \alpha - 1 \leq I(G,\alpha) \leq \log\left(n - 3 + 2^{2+\alpha}\right) - 2\alpha\log(n-1) - 1.$$

(ii) Let T be a tree with n vertices. For $\alpha \in [-1/2, 0]$, we have:

$$(\alpha+1)\log(n-1)-\alpha \leq I(G,\alpha) \leq \log(1+(n-3)2^{\alpha-1})-2\alpha\log(n-1)+\alpha+1;$$

for $\alpha \in [-\infty, -2]$, when n is odd, we have:

$$(\alpha+1)\log(n-1)-\alpha \leq I(G,\alpha) \leq \log\left((n-1)^{\alpha}+2^{\alpha}\right)+(1-2\alpha)\log(n-1)-1,$$

when n is even, we have:

$$(\alpha+1)\log(n-1)-\alpha \leq I(G,\alpha) \leq \log\left(\frac{n-2}{2}((n-2)^{\alpha}+2^{\alpha})+4^{\alpha}\right)-2\alpha\log(n-1).$$

Corollary 2. *Let G be a simple connected graph with n vertices. Then:*

$$\log\left(\frac{1}{2}\sum_{i=1}^{n} d_i^{2\alpha+1}-\frac{k}{2}\lambda_1(G)\right)-\alpha \leq I(G,\alpha) \leq \log\left(\frac{1}{2}\sum_{i=1}^{n} d_i^{2\alpha+1}-\frac{k}{2}\lambda_{n-1}(G)\right)-2\alpha\log(n-1),$$

where $k=\sum\limits_{i=1}^{n} d_i^{2\alpha}-\frac{1}{n}(\sum_{i=1}^{n} d_i^{\alpha})^2$.

From the proof of Theorem 2, we get the following result.

Corollary 3. *Let G be a graph with n vertices. Let δ and Δ be the minimum degree and the maximum degree of G, respectively. Then, for $\alpha < 0$, we have:*

$$\log(R')-2\alpha\log(\delta) \leq I(G,\alpha) \leq \log(R)-2\alpha\log(\Delta),$$

where $R'=\min R_{\alpha}(G)$ and $R=\max R_{\alpha}(G)$.

In the following, we will study some extremal properties of $I(G,\alpha)$ for some classes of graphs.

Theorem 3. *Let $G=(V,E,w)$ be a regular graph with n vertices and $n \geq 3$. Then, we have:*

$$\log n \leq I(G,\alpha) \leq \log\left(\frac{n(n-1)}{2}\right).$$

The left equality holds if and only if G is the cycle graph, and the right equality holds if and only if G is the complete graph.

Proof. Suppose $G=(V,E,w)$ is k-regular. Then, $k \geq 2$, since G is connected and $n \geq 3$. Therefore, we have:

$$I(G,\alpha)=-\sum_{e\in E}\frac{k^{2\alpha}}{\sum_{e\in E}k^{2\alpha}}\log\frac{k^{2\alpha}}{\sum_{e\in E}k^{2\alpha}}=\log\frac{nk}{2}.$$

Since $2 \leq k \leq n-1$, we have:

$$\log n \leq I(G,\alpha) \leq \log\left(\frac{n(n-1)}{2}\right).$$

The proof is complete. □

In the following, we prove bounds for complete bipartite graphs. However, it seems not easy to determine bounds for the complete k-partite graphs.

Theorem 4. *Let $G = (V, E, w)$ be a complete bipartite graph with n vertices. Then, we infer:*

$$\log(n-1) \leq I(G, \alpha) \leq \log\left(\left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil\right).$$

The left equality holds if and only if G is the star graph, and the right equality holds if and only if G is the balanced complete bipartite graph.

Proof. Suppose $G = (V, E, w)$ is a complete bipartite graph with n vertices, and the two parts have p and q vertices, respectively. Therefore, $p + q = n$. We have:

$$I(G, \alpha) = -\sum_{e \in E} \frac{(pq)^\alpha}{\sum_{e \in E}(pq)^\alpha} \log \frac{(pq)^\alpha}{\sum_{e \in E}(pq)^\alpha} = \log(pq).$$

Thus,

$$\log(n-1) \leq I(G, \alpha) \leq \log\left(\left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil\right).$$

The left equality holds if and only if $p = 1$ and $q = n - 1$, *i.e.*, G is a star. The right equality holds if and only if $p = \left\lfloor \frac{n}{2} \right\rfloor$ and $q = \left\lceil \frac{n}{2} \right\rceil$, *i.e.*, G is the balanced complete bipartite graph. $\square$

A comet is a tree composed of a star and a pendent path. For any numbers n and $2 \leq t \leq n-1$, we denote by $CS(n, t)$ the comet of order n with t pendent vertices, *i.e.*, a tree formed by a path P_{n-t} of which one end vertex coincides with a pendent vertex of a star S_{t+1} of order $t+1$. Observe that $CS(n, t)$ is the path graph if $t = 2$ and is the star graph if $t = n - 1$. Then, for $2 \leq t \leq n - 2$, we have:

$$\begin{aligned} I(CS(n,t), \alpha) = &\log\left(2^\alpha + (2t)^\alpha + (t-1)t^\alpha + (n-t-2)4^\alpha\right) \\ &- \frac{\alpha\left(2^\alpha + (2t)^\alpha \log(2t) + (t-1)t^\alpha \log t + 2(n-t-2)4^\alpha\right)}{2^\alpha + (2t)^\alpha + (t-1)t^\alpha + (n-t-2)4^\alpha}. \end{aligned}$$

By some elementary calculations, we get the following result.

Theorem 5. *Among all comets with n vertices and parameter t,*
(i) for $\alpha = 1$, we have:

$$I(CS(n, t_0), \alpha) \leq I(CS(n,t), \alpha) \leq \log(n-1),$$

the right equality holds if and only if $t = n - 1$, i.e., $CS(n, t)$ is the star graph, and the left equality holds if and only if $t = t_0$, where $t_0 \geq 3$ is the root the equation $\frac{\partial I(CS(n,t),1)}{\partial t} = 0$, i.e.,

$$((t^2+t)\log t - 6t + 8n - 14)(2t-3) = (t^2 - 3t + 4n - 6)((2t+1)\log t - \frac{t-4}{\ln 2} - 6).$$

(ii) For $\alpha = -1$, we have:

$$I(CS(n,t), \alpha) \leq \log(n-1),$$

the right equality holds if and only if $t = n - 1$, i.e., $CS(n, t)$ is the star graph, and the left equality holds if and only if $t = t_0'$, where $t_0' \geq 4$ is the root the equation $\frac{\partial I(CS(n,t),-1)}{\partial t} = 0$, i.e.,

$$(1 + (2t-1)\log t + (n-t)t)(2 - t^2) = (2t - 1 + \frac{(n-t)t}{2})(-2 - 2t^2 + 2\log t + \frac{4t - t^2}{\ln 2}).$$

By performing a numerical study, we also list some values of t_0 and t'_0 as follows in Table 1.

Table 1. Some values of t_0 and t'_0.

n		**30**	**40**	**50**	**60**	**100**	**200**	**300**	**400**	**500**	**1000**
t_0	11	15	19	22	25	36	57	74	88	102	155
t'_0	18	27	36	45	54	92	190	288	387	486	983

For most of the topological indices on trees with a given number of vertices, we obtain that the star graph and the path graph are the extremal graphs maximal or minimal values. However, from Theorem 5, the path graph is not the extremal graph among all trees, as the path graph is also a comet. It seems to be intricate to determine extremal values of this entropy and to characterize the corresponding extremal graphs among all trees with a given number of vertices for any real number α.

Similarly, by some elementary calculations, we get the extremal values of double stars.

Theorem 6. *For $S_{p,q}$, we have that for $\alpha \in [0.5, +\infty)$,*

$$I(S_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}, \alpha) \leq I(S_{p,q}, \alpha) \leq I(S_{1,n-1}, \alpha);$$

for $\alpha \in [-\infty, -0.5)$,

$$I(S_{1,n-1}, \alpha) \leq I(S_{p,q}, \alpha) \leq I(S_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}, \alpha).$$

We try to determine the bounds for all values of α. However, the problem seems quite complicated when $\alpha \in (-0.5, 0.5)$.

In [20,60], the authors studied the extremal values of entropy based on different well-known information functionals for dendrimers, which possess interesting applications in structural chemistry and computational biology. We also consider the value of $I(G, \alpha)$ for dendrimers.

A dendrimer is a tree with two additional parameters; the progressive degree t and the radius r. Every internal node of the tree has degree $t+1$. As in every tree, a dendrimer has one (monocentric dendrimer) or two (dicentric dendrimer) central nodes; the radius r denotes the (largest) distance from an external node to the (closer) center. If all external nodes are at a distance r from the center, then the dendrimer is called homogeneous. Internal nodes different from the central nodes are called branching nodes and are said to be on the i-th orbit if their distance to the (nearer) center is r. Every branching vertex has one incoming edge, as well as t outgoing edges.

Let $D(t, r)$ denote the dendrimer graph with parameters t and r. If $D(t, r)$ has only one center, then we have $n = 1 + \frac{(t+1)(t^r-1)}{t-1}$. If $D(t, r)$ has only two centers, then we have $n = \frac{2(t^{r+1}-1)}{t-1}$. Observe that $1 \leq t \leq n-2$ and $1 \leq r \leq \lfloor \frac{n-1}{2} \rfloor$. As an example, we show dendrimers with one center (left) and two centers (right), such that t =3 and $r = 3$ in Figure 1. In addition, the graph is the star if $r = 1$ and $t = n-2$, while the graph is the path if $r = \lfloor \frac{n-1}{2} \rfloor$ and $t = 1$. In the following, we suppose $D(t, r)$ has only one center, since the other case is similar. We will show that for $\alpha \in (-\infty, 0)$, the star graph and the path graph attain the minimum and maximum value of $I(G, \alpha)$, respectively. However, it seems very complicated getting such results for $\alpha \in (0, \infty)$.

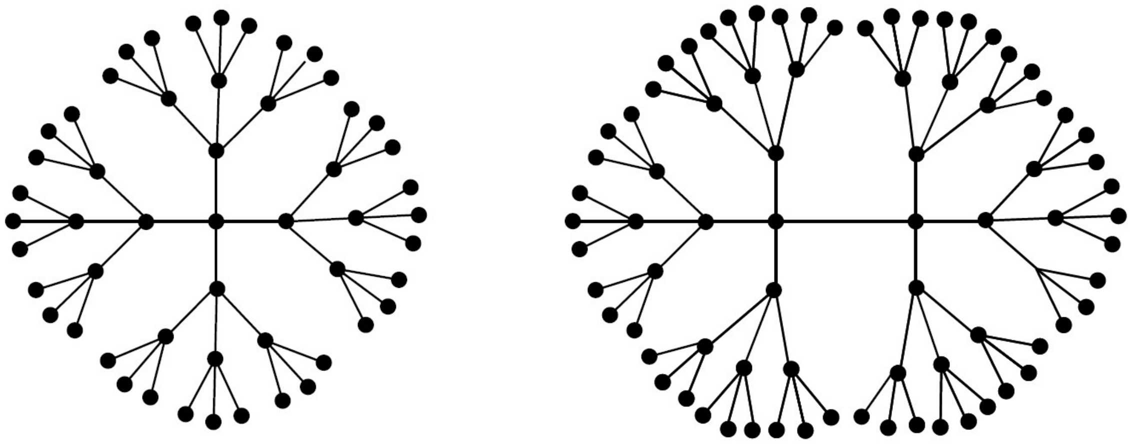

Figure 1. The dendrimers with one center (left) and two centers (right), such that t =3 and $r = 3$.

Theorem 7. *Let $D(t, r)$ be a dendrimer with n vertices with only one center. Then, for $\alpha \in (-\infty, 0)$, we have:*

$$\log\left(2 + (n-3)2^{\alpha}\right) - \frac{\alpha(n-3)2^{\alpha-1}}{1 + (n-3)2^{\alpha-1}} \leq I(G, \alpha) \leq \log(n-1),$$

the left equality holds if and only if $D(t, r)$ is the path graph, and the right equality holds if and only if $D(t, r)$ is the star graph.

Proof. If $r = 1$, *i.e.*, D is a star, then we have $I(D, \alpha) = \log(t + 1)$. Since $D(t, r)$ has only one center, we have $n = 1 + \frac{(t+1)(t^r-1)}{t-1} = t+2$, *i.e.*, $t = n-2$. Therefore, in this case, we have $I(D, \alpha) = \log(n-1)$. If $t = 1$, *i.e.*, D is a path, then by some elementary calculations, we have:

$$I(D, \alpha) = \log\left(2 + (n-3)2^{\alpha}\right) - \frac{\alpha(n-3)2^{\alpha-1}}{1 + (n-3)2^{\alpha-1}}.$$

In the following, we suppose $t \geq 2$, *i.e.*, $r \leq \lfloor \frac{n-1}{2} \rfloor - 1$. Since $D(t, r)$ has only one center, then there are $(t + 1)t^{r-1}$ leaves, and both end vertices of any other edge have degree $t + 1$. Set $A_1 = \sum_{uv\in E} \frac{(d(u)d(v))^{\alpha}}{\sum_{uv\in E}(d(u)d(v))^{\alpha}}$. Then, we infer:

$$\begin{aligned} A_1 &= (t+1)t^{r-1}(t+1)^{\alpha} + (n - 1 - (t+1)t^{r-1})(t+1)^{2\alpha} \\ &= (t+1)t^{r-1}(t+1)^{\alpha} + \frac{t+1}{t-1}(t^{r-1} - 1)(t+1)^{2\alpha}. \end{aligned}$$

Therefore,

$$\begin{aligned} & I(D, \alpha) \\ = & -(t+1)t^{r-1} \cdot \frac{(t+1)^{\alpha}}{A_1} \cdot \log\left(\frac{(t+1)^{\alpha}}{A_1}\right) - (n - 1 - (t+1)t^{r-1}) \cdot \frac{(t+1)^{2\alpha}}{A_1} \cdot \log\left(\frac{(t+1)^{2\alpha}}{A_1}\right) \\ = & -(t+1)t^{r-1} \cdot \frac{(t+1)^{\alpha}}{A_1} \cdot \log\left(\frac{(t+1)^{\alpha}}{A_1}\right) - \frac{t+1}{t-1}(t^{r-1} - 1) \cdot \frac{(t+1)^{2\alpha}}{A_1} \cdot \log\left(\frac{(t+1)^{2\alpha}}{A_1}\right) \\ = & \log\left(t^{r-1}(t+1) + \frac{t+1}{t-1}(t^{r-1} - 1)(t+1)^{\alpha}\right) - \frac{\alpha(t^{r-1} - 1)(t+1)^{\alpha}\log(t+1)}{t^{r-1}(t-1) + (t^{r-1} - 1)(t+1)^{\alpha}}. \end{aligned}$$

By substituting $n = 1 + \frac{(t+1)(t^r-1)}{t-1}$ into the above equality, we have:

$$I(D,\alpha) = \log\left[\frac{nt-n-2}{t} + \frac{(-t^2+(n-1)t-n-2)(t+1)^\alpha}{t(t-1)}\right] - \frac{\alpha(-t^2+(n-1)t-n-2)(t+1)^\alpha \log(t+1)}{(nt-n-2)(t+1)+(-t^2+(n-1)t-n-2)(t+1)^\alpha}.$$

By some elementary calculations, we infer that for $\alpha < 0$ and a given n, $I(D,\alpha)$ is an increasing function on t. Thus, $I(D,\alpha)$ attains the minimum when $t = 1$ and attains the maximum value when $t = n-2$. Thus, we have completed the proof. $\square$

4. Summary and Conclusions

Based on the contribution of Eagle *et al.* [47] investigating vertex entropies, we introduced in our paper the concept of a graph entropy for weighted graphs. To the best of our knowledge, this problem has received very little attention so far with only a few exceptions, e.g., [61]. We examined extremal properties of our entropy definition for special graph classes. Specifically, in this paper, we placed our emphasis on weighted graphs due to Bollobás and Erdös, which is also called the Randić weight.

As an open problem, it would be interesting to consider the extremal values of $I(D,\alpha)$ among all dendrimers for $\alpha \in (0,\infty)$. Furthermore, it is challenging to determine extremal values of $I(T,\alpha)$ among all trees with n vertices for any real number α. One possible attempt to do this could be based on establishing some graph transformations, which can increase or decrease the values of the entropy. This leads to the formulation of the following open problem.

Problem 1. *Determine extremal values of $I(T,\alpha)$ among all trees with n vertices for any real number α.*

This paper mainly considered edge weights defined by Bollobás and Erdös. For future work, it would be interesting to consider other edge weights of graphs, such as the sum-connectivity weight [62,63] and the atom-bond connectivity (ABC) index [64–66], which are well studied with applications in chemistry. Furthermore, it would be interesting to generalize our definition to (weighted) hypergraphs.

On the other hand, the entropy for vertex-weighted graphs can be defined similarly, which has already been studied extensively; see [17,19].

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Author Contributions

Wrote the paper: Zengqiang Chen, Matthias Dehmer, Frank Emmert-Streib and Yongtang Shi. Did the analysis: Zengqiang Chen, Matthias Dehmer, Frank Emmert-Streib and Yongtang Shi. All authors have read and approved the final manuscript.

Conflicts of Interest

The authors declare no conflict of interest.

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