Some properties on entropies of graphs

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Abstract

Shannon entropies for networks have been widely introduced. Several graph invariants have been used for defining graph entropy measures. Using majorization theory, we obtain some lower and upper bounds on graph entropy measures. Moreover we prove more extremal properties for entropies of graphs.

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. Entropy of networks or graphs was introduced by Rashevsky [34] and Mowshowitz [32] when studying mathematical properties of the information measures. As most of the measures are quite generic, it seems to be straightforward that graph entropy measures have been used successfully in various disciplines, e.g., in pattern recognition, biology, chemistry, and computer science, see [1,4,8,16,25,29,30,33,37,38]. Another example is the Körner entropy [28,36] introduced from an information theory-specific point of view when he studied some problem in coding theory.

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Several graph invariants have been used for defining graph entropy measures, such as the number of vertices, vertex degree sequences, extended degree sequences (i.e., the second neighbor, third neighbor, etc.), eigenvalues and other roots of graph polynomials [9, 11, 14, 20, 21, 23]. Distance-based graph entropies [11, 14] have also been studied. In [7], Cao et al. studied properties of graph entropies based on an information functional by using degree powers of graphs and now this entropy measure has been further studied and explored [5, 12, 13]. Note that Dehmer et al. [17] and Emmert-Streib et al. [24] used graph entropies for applications when it comes to define graph distance or similarity measures. In [10, 27], the authors studied the entropy of weighted graphs. Very recently, Cao et al. [6] introduced a new graph entropy based on the number of independent sets and matchings of graphs. Highlights of the recent developments regarding graph entropy can be found in [15].

In this paper, we study more properties of entropies of graphs. Throughout this paper, we are concerned with simple connected graphs. Let $G = (V, E)$ be a simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$, where $|V(G)| = n$ and $|E(G)| = m$. Let d_i be the degree of vertex v_i for $i = 1, 2, \ldots, n$. The maximum and minimum vertex degrees are denoted by Δ and δ, respectively. The *distance* between two vertices $v_i, v_j \in V(G)$, denoted by $d_G(v_i, v_j)$, is defined as the length of a shortest path between v_i and v_j in G. For $v_i \in V(G)$, let $e_G(v_i)$ be the *eccentricity* of the vertex v_i in G, which is defined as $e_G(v_i) = \max\{d_G(v_i, v_j) : v_j \in V(G)\}$. Moreover, $r \leq e_G(v_i) \leq d$ $(1 \leq i \leq n)$, where r and d are the radius and diameter of graph G, respectively.

As usual, K_n, $K_{1,n-1}$ and P_n are respectively, complete graph, star graph and path graph on n vertices. Denote by $DS_{p,q}$ $(p+q+2 = n)$, a double star obtained by adding an edge between two centers of $K_{1,p}$ and $K_{1,q}$. Denoted by $C_{n,2} = DS_{n-3,1}$.

The rest of the paper is structured as follows. In Section 2, we state definitions and related theorems from theory of majorization, needed for the subsequent considerations. In Section 3, we present more properties of entropies of graphs. In Section 4, for trees, we prove an extremal result of the entropy based on degree powers.

2 Preliminaries

Throughout the paper all logarithms have base 2. In the following, we introduce entropy measures studied in this paper and state some preliminaries [14, 19]. All measures examined in this paper are based on Shannon's entropy.

Definition 2.1 *Let $p = (p_1,\, p_2, \ldots,\, p_n)$ be a probability vector, namely, $0 \le p_i \le 1$ and $\sum\limits_{i=1}^{n} p_i = 1$. The Shannon's entropy of p is defined as*

$$I(p) = -\sum_{i=1}^{n} p_i \,\log\, p_i.$$

To define information-theoretic graph measures, we often consider a tuple $(\lambda_1,\, \lambda_2, \ldots,\, \lambda_n)$ of non-negative integers $\lambda_i \in N$ [14]. This tuple forms a probability distribution $p = (p_1,\, p_2, \ldots,\, p_n)$, where

$$p_i = \frac{\lambda_i}{\sum\limits_{j=1}^{n} \lambda_j}, \quad i = 1,\, 2, \ldots,\, n.$$

Therefore, the entropy of tuple $(\lambda_1,\, \lambda_2, \ldots,\, \lambda_n)$ is given by

$$I(\lambda_1,\, \lambda_2, \ldots,\, \lambda_n) = -\sum_{i=1}^{n} p_i \,\log\, p_i = \log\left(\sum_{i=1}^{n} \lambda_i\right) - \sum_{i=1}^{n} \frac{\lambda_i}{\sum\limits_{j=1}^{n} \lambda_j} \,\log\, \lambda_i.$$

In the literature, there are various ways to obtain the tuple $(\lambda_1,\, \lambda_2, \ldots,\, \lambda_n)$, like the so-called magnitude-based information measures introduced by Bonchev and Trinajstić [2], or partition-independent graph entropies, introduced by Dehmer [14,22], which are based on information functionals.

We now introduce two definitions and one theorem from the theory of majorization. Throughout this paper, we consider nonincreasing arrangement of each vector in $\mathbb{R}^n$, that is, for any $x = (x_1, \ldots, x_n) \in \mathbb{R}^n$, we consider $x_1 \ge x_2 \ge \cdots \ge x_n$. With considering this arrangement on vectors x and $y \in \mathbb{R}^n$, the following definitions are given in [31].

Definition 2.2 [31] *For $x,\, y \in \mathbb{R}^n$, $x \prec y$ if*

$$\begin{cases} \sum\limits_{i=1}^{k} x_i \leq \sum\limits_{i=1}^{k} y_i, & k = 1,\, 2, \ldots,\, n-1, \\ \\ \sum\limits_{i=1}^{n} x_i = \sum\limits_{i=1}^{n} y_i. \end{cases}$$

When $x \prec y$, x is said to be majorized by y (y majorizes x).

Definition 2.3 [31] *For $x,\, y \in \mathbb{R}^n$, $x \prec_W y$ if*

$$\sum_{i=1}^{k} x_i \leq \sum_{i=1}^{k} y_i, \qquad k = 1,\, 2, \ldots,\, n,$$

and $x \prec^W y$ if

$$\sum_{i=1}^{k} x_{n+1-i} \geq \sum_{i=1}^{k} y_{n+1-i}, \qquad k = 1,\, 2, \ldots,\, n.$$

In either case, x is said to be weakly majorized by y (y weakly majorizes x). More specifically, x is said to be weakly submajorized by y if $x \prec_W y$ and x is said to be weakly supermajorized by y if $x \prec^W y$. Alternatively, we say weakly majorized from below or weakly majorized from above, respectively.

The following theorem is given in (p. 165, [31]).

Theorem 2.4 [31] *For all convex functions g,*

$$x \prec y \;\Rightarrow\; (g(x_1),\, \ldots,\, g(x_n)) \prec_W (g(y_1),\, \ldots,\, g(y_n)); \tag{2.1}$$

and for all concave functions g,

$$x \prec y \;\Rightarrow\; (g(x_1),\, \ldots,\, g(x_n)) \prec^W (g(y_1),\, \ldots,\, g(y_n)). \tag{2.2}$$

3 Some results on entropy of graphs

In this section we label the vertices in graph G such that $e_G(v_1) \geq e_G(v_2) \geq \cdots \geq e_G(v_n)$, where $e_G(v_i)$ is the eccentricity of v_i in G. We define $p_i = \frac{e_G(v_i)}{\sum\limits_{j=1}^{n} e_G(v_j)}$. Therefore, the entropy is given by

$$I(G) = -\sum_{i=1}^{n} \frac{e_G(v_i)}{\sum\limits_{j=1}^{n} e_G(v_j)} \log \left(\frac{e_G(v_i)}{\sum\limits_{j=1}^{n} e_G(v_j)} \right).$$

Denote by

$$e_G = \left(\frac{e_G(v_1)}{\sum\limits_{j=1}^{n} e_G(v_j)}, \frac{e_G(v_2)}{\sum\limits_{j=1}^{n} e_G(v_j)}, \ldots, \frac{e_G(v_n)}{\sum\limits_{j=1}^{n} e_G(v_j)} \right).$$

We now give a theorem related to majorization.

Theorem 3.1 *Let H and G be two non-isomorphic graphs of order n such that $e_H \prec e_G$. Then $I(G) \leq I(H)$.*

Proof: Let us consider a function $g(x) = -x \log x$. Then we have $g''(x) = -\frac{1}{x \ln 2} < 0$ for any $x > 0$. Therefore $g(x_i)$ is a concave function for $x_i > 0$. Now,

$$I(G) = -\sum_{i=1}^{n} x_i \log x_i,$$

where $x_i = \frac{e_G(v_i)}{\sum\limits_{j=1}^{n} e_G(v_j)} > 0$. Since $e_H \prec e_G$, by Theorem 2.4 with the above entropy definition, we have

$$I(G) = -\sum_{i=1}^{n} \frac{e_G(v_i)}{\sum\limits_{j=1}^{n} e_G(v_j)} \log \frac{e_G(v_i)}{\sum\limits_{j=1}^{n} e_G(v_j)} \leq -\sum_{i=1}^{n} \frac{e_H(v_i)}{\sum\limits_{j=1}^{n} e_H(v_j)} \log \frac{e_H(v_i)}{\sum\limits_{j=1}^{n} e_H(v_j)} = I(H).$$

∎

Example 3.2 *The two non-isomorphic trees H_1 and H_2 have been shown in Fig. 1. We have*

$$e_{H_1} = \left(\frac{6}{53}, \frac{6}{53}, \frac{6}{53}, \frac{6}{53}, \frac{5}{53}, \frac{5}{53}, \frac{4}{53}, \frac{4}{53}, \frac{4}{53}, \frac{4}{53}, \frac{3}{53} \right)$$

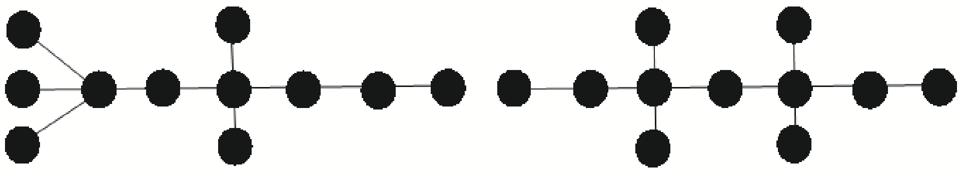
and

$$e_{H_2} = \left(\frac{6}{53}, \frac{6}{53}, \frac{5}{53}, \frac{5}{53}, \frac{5}{53}, \frac{5}{53}, \frac{5}{53}, \frac{5}{53}, \frac{4}{53}, \frac{4}{53}, \frac{3}{53} \right).$$

Then, we have

$$\sum_{j=1}^{n} e_{H_1}(v_j) = \sum_{j=1}^{n} e_{H_2}(v_j) = 1.$$

One can easily see that $e_{H_2} \prec e_{H_1}$. Moreover, $I(H_1) < I(H_2)$ by direct checking. By the above theorem, we have $I(H_1) \leq I(H_2)$.



H_1 H_2

Fig. 1. Trees H_1 and H_2.

Remark 3.3 *Dehmer et al. [18] mentioned that $I(C_{n,2}) > I(K_{1,n-1})$. We have $e_{C_{n,2}} = \Big(\underbrace{\frac{3}{3n-2}, \ldots, \frac{3}{3n-2}}_{n-2}, \frac{2}{3n-2}, \frac{2}{3n-2}\Big)$ and $e_{K_{1,n-1}} = \Big(\underbrace{\frac{2}{2n-1}, \ldots, \frac{2}{2n-1}}_{n-1}, \frac{1}{2n-1}\Big)$. Since*

$$\frac{e_{C_{n,2}}(v_1)}{\sum_{j=1}^{n} e_{C_{n,2}}(v_j)} = \frac{3}{3n-2} > \frac{2}{2n-1} = \frac{e_{K_{1,n-1}}(v_1)}{\sum_{j=1}^{n} e_{K_{1,n-1}}(v_j)}$$

and

$$\sum_{i=1}^{n-1} \frac{e_{C_{n,2}}(v_i)}{\sum_{j=1}^{n} e_{C_{n,2}}(v_j)} = \frac{3n-4}{3n-2} < \frac{2(n-1)}{2n-1} = \sum_{i=1}^{n-1} \frac{e_{K_{1,n-1}}(v_i)}{\sum_{j=1}^{n} e_{K_{1,n-1}}(v_j)},$$

we have that $e_{C_{n,2}} \not\prec e_{K_{1,n-1}}$ and $e_{K_{1,n-1}} \not\prec e_{C_{n,2}}$. But we have $I(C_{n,2}) > I(K_{1,n-1})$.

Remark 3.4 *Again in [18], Dehmer et al. conjectured that the comet $C_{n,2}$ has maximal entropy among all trees of order n. Since several other trees have the same value of entropy as $C_{n,2}$, the above statement is not correct. We have $e_{DS_{p,q}} = e_{C_{n,2}}$. Then the conjecture should be the following: the double star $DS_{p,q}$ has maximal entropy among all trees of order n or $I(T) \leq I(C_{n,2}) = I(DS_{p,q})$ with equality holding if and only if $T \cong DS_{p,q}$ $(p+q+2=n)$.*

Theorem 3.5 *Let T be a tree of order n. Then*

$$\frac{e_T(v_n)}{\sum_{j=1}^{n} e_T(v_j)} \geq \frac{1}{2n-1} \tag{3.1}$$

with equality holding if and only if $T \cong K_{1,\,n-1}$.

Proof: If $T \cong K_{1,\,n-1}$, then the equality holds in (3.1). Otherwise, $T \ncong K_{1,\,n-1}$. Since $d = e_T(v_1) \geq e_T(v_2) \geq \cdots \geq e_T(v_n) = r$ and $d \leq 2r$, we have $e_T(v_k) - e_T(v_n) \leq r = e_T(v_n)$, $k = 1,\, 2, \ldots,\, n$. Then

$$\sum_{k=1}^{n-1} \left(e_T(v_k) - e_T(v_n)\right) \leq (n-1)\, e_T(v_n), \text{ that is, } \sum_{k=1}^{n} e_T(v_k) \leq (2n-1)\, e_T(v_n).$$

The first part of the proof is done.

Let v_n be the center of the tree T such that $e_T(v_n) = r$. Since $T \ncong K_{1,\,n-1}$, then $r \geq 2$. Then there exists a non-pendant vertex v_j in T such that $v_n v_j \in E(T)$. Therefore $e_T(v_j) - e_T(v_n) \leq 1 < r$ and hence the inequality in (3.1) is strict. ∎

The *center* $C(G)$ of a graph G is the set of vertices with minimum eccentricity. A graph G is *self-centered* (SC) if all its vertices lie in the center $C(G)$. For more results on self-centered graphs, we refer to [3]. Thus, the eccentric set of a self-centered graph contains only one element, that is, all the vertices have the same eccentricity. Equivalently, a self-centered graph is a graph whose diameter equals its radius.

Theorem 3.6 *Let* G *be a self-centered graph of order* n. *Then we have* $I(G) = \log n \geq I(K_{1,\,n-1})$.

Proof: For a self-centered graph G, $e_G(v_1) = e_G(v_2) = \cdots = e_G(v_n)$. Then we have

$$I(G) = -\sum_{i=1}^{n} \frac{1}{n} \log \left(\frac{1}{n}\right) = \log n.$$

Since $I(K_{1,\,n-1}) = \log(2n-1) - \frac{2(n-1)}{2n-1}$, we have to prove that

$$\log n \geq \log(2n-1) - \frac{2(n-1)}{2n-1}, \text{ that is, } 1 - \frac{1}{2n-1} \geq \log\left(2 - \frac{1}{n}\right).$$

Let $f(x) = 1 - \frac{1}{2x-1} - \log\left(2 - \frac{1}{x}\right)$. By some elementary calculations, we have

$$f'(x) = \frac{1}{2x-1}\left(\frac{2}{2x-1} - \frac{1}{x \ln 2}\right).$$

Since $\frac{2}{2x-1} < \frac{1}{x\ln 2}$ for $x \geq 2$, we have $f'(x) < 0$ for $x \geq 2$, which implies that $f(n)$ is a decreasing function on $n \geq 2$. Since when $n \to \infty$,

$$\frac{1}{2} > \left(1 - \frac{1}{2n}\right)^{2n} \frac{2n}{2n-1}, \quad \text{that is, } 2^{-\frac{1}{2n-1}} > 1 - \frac{1}{2n},$$

we have $f(+\infty) > 0$. Therefore, we have $f(n) \geq f(+\infty) > 0$. The proof is thus complete. ∎

Lemma 3.7 *Let G be a graph of order n. Then*

$$\frac{e_G(v_1)}{\sum\limits_{j=1}^{n} e_G(v_j)} \geq \frac{1}{n} \quad \text{and} \quad \frac{e_G(v_n)}{\sum\limits_{j=1}^{n} e_G(v_j)} \leq \frac{1}{n} \tag{3.2}$$

with both equalities hold if and only if $G \cong SC$.

Proof: Since

$$e_G(v_1) \geq e_G(v_2) \geq \cdots \geq e_G(v_n) \quad \text{and} \quad \sum_{i=1}^{n} \frac{e_G(v_i)}{\sum\limits_{j=1}^{n} e_G(v_j)} = 1,$$

we get the required result in (3.2). Moreover, both equalities hold if and only if $e_G(v_1) = e_G(v_2) = \cdots = e_G(v_n)$, that is, $G \cong SC$. ∎

In [9], Chen et al. studied the maximal and minimal entropy for dendrimers. Here we obtain the following result for any graph G.

Theorem 3.8 *Let G be a graph of order n. Then $I(G) \leq I(SC)$.*

Proof: First we have to prove that

$$\sum_{i=1}^{k} \frac{e_G(v_i)}{\sum\limits_{j=1}^{n} e_G(v_j)} \geq \frac{k}{n}\,. \tag{3.3}$$

By (3.2), the result in (3.3) holds for $k = 1$ and $k = n-1$. For $k = n$, the equality holds in (3.3). By contradiction we have to prove that the result in (3.3) holds for any k, $2 \leq k \leq n-2$. For this we assume that there exists a smallest positive integer p ($p \leq n-2$) such that

$$\sum_{i=1}^{p} \frac{e_G(v_i)}{\sum_{j=1}^{n} e_G(v_j)} < \frac{p}{n}. \tag{3.4}$$

Since

$$e_G(v_1) \geq e_G(v_2) \geq \cdots \geq e_G(v_n),$$

from the above, we must have

$$e_G(v_n) \leq e_G(v_{n-1}) \leq \cdots \leq e_G(v_p) < \frac{1}{n}\,.$$

Using the above result, we get

$$1 = \sum_{i=1}^{n} \frac{e_G(v_i)}{\sum_{j=1}^{n} e_G(v_j)} = \sum_{i=1}^{p} \frac{e_G(v_i)}{\sum_{j=1}^{n} e_G(v_j)} + \sum_{i=p+1}^{n} \frac{e_G(v_i)}{\sum_{j=1}^{n} e_G(v_j)} < \frac{p}{n} + \frac{n-p}{n} = 1,$$

a contradiction. Hence we get the inequality in (3.3) for any k, $1 \leq k \leq n$.

Therefore $e_G \succ e_{SC}$ and hence $I(G) \leq I(SC)$, by Theorem 3.1. ∎

4 More on a conjecture of graph entropy

In this section we can assume that $d_1 \geq d_2 \geq \cdots \geq d_n$ and denote by

$$e_G = \left(\frac{d_1^k}{\sum_{j=1}^{n} d_j^k}, \frac{d_2^k}{\sum_{j=1}^{n} d_j^k}, \ldots, \frac{d_n^k}{\sum_{j=1}^{n} d_j^k} \right).$$

Cao *et al.* [7] introduced the following special graph entropy.

$$I(G) = -\sum_{i=1}^{n} \frac{d_i^k}{\sum_{j=1}^{n} d_j^k} \log \left(\frac{d_i^k}{\sum_{j=1}^{n} d_j^k} \right), \tag{4.1}$$

where d_i is the degree of the vertex v_i in G. According to [20], we see that $\lambda_i = d_i^k$.

A graph G is said to be *r-regular* if all of its vertices have the same degree r. For an r-regular graph G,

$$I(G) = \log n.$$

Lemma 4.1 *Let G be a graph of order n. Then*

$$\frac{d_1^k}{\sum\limits_{j=1}^{n} d_j^k} \geq \frac{1}{n} \quad \text{and} \quad \frac{d_n^k}{\sum\limits_{j=1}^{n} d_j^k} \leq \frac{1}{n} \tag{4.2}$$

with both equalities hold if and only if G is a regular graph.

Proof: Since

$$d_1 \geq d_2 \geq \cdots \geq d_n \quad \text{and} \quad \sum_{i=1}^{n} \frac{d_i^k}{\sum\limits_{j=1}^{n} d_j^k} = 1 = \sum_{i=1}^{n} \frac{1}{n},$$

we get the required result in (4.2). Moreover, both equalities hold if and only if $d_1 = d_2 = \cdots = d_n$, that is, G is a regular graph. ∎

We now give a theorem related to majorization.

Theorem 4.2 *Let H and G be two non-isomorphic graphs of order n such that $e_H \prec e_G$. Then $I(G) \leq I(H)$.*

Proof: The proof is very similar to Theorem 3.1. ∎

We now give an upper bound on $I(G)$ of any graph G.

Theorem 4.3 *Let G be a graph of order n. Then $I(G) \leq I(H) = \log n$, where H is a regular graph of order n.*

Proof: Same proof as in Theorem 3.8. ∎

The following conjecture was proposed in [7] and the upper bound was proved in [13]. Recently, Ilić proved the following conjecture fully [26].

Conjecture 4.4 *Let T be a tree with n vertices and $k > 0$. Then we have $I(T) \leq I(P_n)$, the equality holds if and only if $T \cong P_n$; $I(T) \geq I(S_n)$, the equality holds if and only if $T \cong S_n$.*

Here we give the following result:

Theorem 4.5 *Let T ($\ncong K_{1,n-1}$) be a tree of order n. Then $I(T) \geq I(C_{n,2})$.*

Proof: We have

$$e_{C_{n,2}} = \left(\frac{(n-2)^k}{(n-2)^k + 2^k + n - 2}, \frac{2^k}{(n-2)^k + 2^k + n - 2}, \underbrace{\frac{1}{(n-2)^k + 2^k + n - 2}, \ldots, \frac{1}{(n-2)^k + 2^k + n - 2}}_{n-2} \right) \tag{4.3}$$

We denote by

$$M_k(G) = \sum_{i=1}^{n} d_i^k \quad (k \geq 1).$$

Claim 1. Let T ($\ncong K_{1,n-1}$) be a tree of order n. Then $M_k(T) \leq M_k(C_{n,2}) < M_k(K_{1,n-1})$ ($k \geq 1$ is a positive integer), that is,

$$M_k(T) \leq (n-2)^k + 2^k + n - 2 < (n-1)^k + n - 1. \tag{4.4}$$

Proof of Claim 1: For $T \cong C_{n,2}$, the equality holds in (4.4). Otherwise, $T \ncong K_{1,n-1}, C_{n,2}$, that is, $\Delta \leq n-3$. Let v_1 be the maximum degree vertex in T. Also let v_k be a pendent vertex adjacent to vertex v_j ($j \neq 1$). We use the following transformation:

$$T + v_1 v_k - v_j v_k \rightarrow T^1.$$

Now,

$$M_k(T^1) - M_k(T) = (d_1 + 1)^k - d_1^k - d_j^k + (d_j - 1)^k.$$

Let us consider a function $f(x) = (x+1)^k - x^k$, $x \geq 1$. Then $f(x)$ is an increasing function on x, we have $f(x+1) \geq f(x)$, that is, $M_k(T^1) \geq M_k(T)$. We apply the above transformation several times, finally we obtain the tree $C_{n,2}$. This proves **Claim 1**.

Since $T \ncong K_{1,n-1}$ ($\Delta \leq n-2$), one can easily see that

$$\frac{d_i^k}{\sum_{i=1}^n d_i^k} \leq \frac{(n-2)^k}{(n-2)^k + 2^k + n - 2} < \frac{(n-1)^k}{(n-1)^k + n - 1}. \tag{4.5}$$

Since T is a tree, we have $\sum_{i=3}^n d_i^k \geq n-2$. By **Claim 1**, we get

$$\sum_{i=1}^n d_i^k \leq (n-2)^k + 2^k + n - 2 \leq \left[(n-2)^{k-1} + \frac{2^k}{n-2} + 1\right] \sum_{i=3}^n d_i^k,$$

that is,

$$\frac{\sum_{i=3}^n d_i^k}{\sum_{i=1}^n d_i^k} \geq \frac{n-2}{(n-2)^k + 2^k + n - 2},$$

that is,

$$\frac{d_1^k + d_2^k}{\sum_{i=1}^n d_i^k} \leq \frac{(n-2)^k + 2^k}{(n-2)^k + 2^k + n - 2}. \tag{4.6}$$

Again since $T \ncong K_{1,n-1}$, by **Claim 1**, we have

$$\frac{d_i^k}{\sum_{j=1}^n d_j^k} \geq \frac{1}{(n-2)^k + 2^k + n - 2} \quad \text{for} \quad i = 1, 2, \ldots, n. \tag{4.7}$$

Since

$$\sum_{i=1}^n \frac{d_i^k}{\sum_{j=1}^n d_j^k} = 1$$

with (4.6), (4.7) and (4.3), one can easily see that

$$\sum_{i=1}^p \frac{d_i^k}{\sum_{j=1}^n d_j^k} \leq \frac{(n-2)^k + 2^k + p - 2}{(n-2)^k + 2^k + n - 2}, \; 3 \leq p \leq n.$$

From the above result with (4.5) and (4.6), we conclude that $e_T \prec e_{C_{n,2}}$ and hence $I(T) \geq I(C_{n,2})$, by Theorem 4.2. ∎

5 Conclusion

As reported by Dehmer and Kraus [18], it turned out that determining extremal values of graph entropies for some given classes of graphs is intricate because there is a lack of analytical methods to tackle this particular problem. In this paper, we continue to prove some extremal properties for some entropies of graphs, especially for trees. We believe that our methods can be used to prove some general cases. As a future work, we will try to apply our method to more classes of general graphs.

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References

[1] E. B. Allen, Measuring graph abstractions of software: An information-theory approach, in: Proceedings of the 8-th International Symposium on Software Metrics table of contents, IEEE Computer Society, 2002, p. 182.

[2] D. Bonchev, N. Trinajstić, Information theory, distance matrix and molecular branching, *J. Chem. Phys.* **67** (1977) 4517–4533.

[3] F. Buckley, Self-centered graphs, *Annals of the New York Academy of Sciences* **576 (1)** (1989) 71–78.

[4] J. Cao, M. Shi, L. Feng, On the edge-hyper-hamiltonian laceability of balanced hypercube, *Discuss Math. Graph Theory.* **36** (2016) 805–817

[5] S. Cao, M. Dehmer, Degree-based entropies of networks revisited, *Appl. Math. Comput.* **261** (2015) 141–147.

[6] S. Cao, M. Dehmer, Z. Kang, Network entropies based on independent sets and matchings, *Appl. Math. Comput.*, in press.

[7] S. Cao, M. Dehmer, Y. Shi, Extremality of degree-based graph entropies, *Inform. Sci.* **278** (2014) 22–33.

[8] Y. Chen, K. Wu, X. Chen, C. Tang, Q. Zhu, An entropy-based uncertainty measurement approach in neighborhood systems, *Inform. Sci.* **279** (2014) 239–250.

[9] Z. Chen, M. Dehmer, F. Emmert-Streib, Y. Shi, Entropy bounds for dendrimers, *Appl. Math. Comput.* **242** (2014) 462–472.

[10] Z. Chen, M. Dehmer, F. Emmert-Streib, Y. Shi, Entropy of weighted graphs with Randić weights, *Entropy* **17 (6)** (2015) 3710–3723.

[11] Z. Chen, M. Dehmer, Y. Shi, A note on distance-based graph entropies, *Entropy* **16 (10)** (2014) 5416–5427.

[12] Z. Chen, M. Dehmer, Y. Shi, Bounds for degree-based network entropies, *Appl. Math. Comput.* **265** (2015) 983–993.

[13] K. C. Das, M. Dehmer, A conjecture regarding the extremal values of graph entropy based on degree powers, *Entropy* **18 (5)** (2016) 183.

[14] M. Dehmer, Information processing in complex networks: Graph entropy and information functionals, *Appl. Math. Comput.* **201** (2008) 82–94.

[15] M. Dehmer, F. Emmert-Streib, Z. Chen, X. Li, Y. Shi, *Mathematical Foundations and Applications of Graph Entropy*, Wiley-Blackwell, 2016.

[16] M. Dehmer, F. Emmert-Streib, M. Grabner, A computational approach to construct a multivariate complete graph invariant, *Inform. Sci.* **260** (2014) 200–208.

[17] M. Dehmer, F. Emmert-Streib, Y. Shi, Interrelations of graph distance measures based on topological indices, *PLoS ONE* **9** (2014), e94985.

[18] M. Dehmer, V. Kraus, On extremal properties of graph entropies, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 889–912.

[19] M. Dehmer, A. Mowshowitz, Inequalities for entropy-based measures of network information content, *Appl. Math. Comput.* **215** (2010) 4263–4271.

[20] M. Dehmer, A. Mowshowitz, A history of graph entropy measures, *Inform. Sci.* **181** (2011) 57–78.

[21] M. Dehmer, A. Mowshowitz, Y. Shi, Structural differentiation of graphs using Hosoya-based indices, *PLoS ONE* **9 (7)** (2014), e102459.

[22] M. Dehmer, K. Varmuza, S. Borgert, F. Emmert-Streib, On entropy-based molecular descriptors: statistical analysis of real and synthetic chemical structures, *J. Chem. Inf. Model.* **49** (2009) 1655–1663.

[23] S. Dragomir, C. Goh, Some bounds on entropy measures in information theory, *Appl. Math. Lett.* **10** (1997) 23–28.

[24] F. Emmert-Streib, M. Dehmer, Y. Shi, Fifty years of graph matching, network alignment and comparison, *Inform. Sci.* **346–347** (2016) 180–197.

[25] L. Feng, J. Cao, W. Liu, S. Ding, H. Liu, The spectral radius of edge chromatic critical graphs, *Linear Algebra Appl.* **492** (2016) 78–88.

[26] A. Ilić, On the extremal values of general degree-based graph entropies, *Inform. Sci.* **370–371** (2016) 424–427.

[27] R. Kazemi, Entropy of weighted graphs with the degree-based topological indices as weights, *MATCH Commun. Math. Comput. Chem.* **76** (2016) 69–80.

[28] J. Körner, Coding of an information source having ambiguous alphabet and the entropy of graphs, Transactions of the 6-th Prague Conference on Information Theory (1973) 411–425.

[29] V. Kraus, M. Dehmer, F. Emmert-Streib, Probabilistic inequalities for evaluating structural network measures, *Inform. Sci.* **288** (2014) 220–245.

[30] G. Lawyer, Understanding the influence of all nodes in a network, *Sci. Rep.* **5** (2015), 8665.

[31] A.W. Marshall, I. Olkin, B.C. Arnold, *Inequalities: Theory of Majorization and Its Applications*, Second edition, Springer-Verlag, New York, 2011.

[32] A. Mowshowitz, Entropy and the complexity of the graphs I: An index of the relative complexity of a graph, *Bull. Math. Biophys.* **30** (1968) 175–204.

[33] A. Mowshowitz, M. Dehmer, Entropy and the complexity of graphs revisited, *Entropy* **14 (3)** (2012) 559–570.

[34] N. Rashevsky, Life, information theory, and topology, *Bull. Math. Biophys.* **17** (1955) 229–235.

[35] C.E. Shannon, W. Weaver, W. *The Mathematical Theory of Communication*, University of Illinois Press: Urbana, IL, USA, 1949.

[36] G. Simonyi, Graph entropy: A survey, Combinatorial Optimization, *DIMACS Ser. Discr. Math. Theor. Comput. Sci.* **20** (1995) 399–441.

[37] X. Yang, W. Liu, H. Liu, L. Feng, Incidence graphs constructed from t-designs, *Appl. Anal. Discrete Math.* **10** (2016) 457–478.

[38] G. Yu, X. Liu, H. Qu, Singularity of Hermitian (quasi-)Laplacian matrix of mixed graphs, *Appl. Math. Comput.* **293** (2017) 287–292.