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On Extremal Properties of General Graph Entropies

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Abstract

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 apply the strong mixing variables method for this propose. We characterized the graphs which attain the minimum values of the graph entropy, based on an arbitrary increasing convex information functional, among certain classes of graphs, namely, trees, unicyclic graphs and bicyclic graphs.

1 Introduction

In the last fifty years, the investigations into the information content of graphs and networks have been based on the profound and initial works due to Shannon [24, 25]. In order to measure the structural complexity of graphs and networks, the concept of graph entropy has been proposed [23, 26]. Determining the complexity of the graphs, has been used in various filed of sciences, including information theory, biology, chemistry and sociology [1, 2, 9, 11].

However, there is still no general accepted description of the complexity of a graph that would allow the foundation of a quantitative measure for its characterization. Therefore, various types of graph entropies are present in scientific articles. For extensive overview on graph entropy measures and statistical analysis of topological graph measures we refer the reader to [14] and [18], respectively. The definition of graph entropy, by using an arbitrary information functional, is due to Dehmer [12, 13].

Incidentally, let $G = (V(G), E(G)$ be a connected simple graph and S be a certain set of associated objects of G. Then a monotonous function $f : S \to \mathbb{R}_+$ is called an information functional of G. In addition, the corresponding entropy of G is defined as:

$$I_f(G) = -\sum_{i=1}^{|S|} \frac{f(s_i)}{\sum_{j=1}^{|S|} f(s_j)} \log\left(\frac{f(s_i)}{\sum_{j=1}^{|S|} f(s_j)}\right).$$

Several sets, such as the sets of all vertices and independent vertices, vertex degree sequence, extended degree sequences (i.e., the second neighbor, third neighbor, etc.), eigenvalues and other roots of graph polynomials, [4–7, 13, 14, 16, 17, 19], have been used for defining I_f.

As reported by Dehmer and Kraus [15], there are very little work to find the extremal values of graph entropies; because Shannon's entropy represents a multivariate function and all probability values are not equal to zero when considering graph entropies [3]. A more studied example of I_f, denoted by I_k in [3], is the case that $S = V(G)$ and $f(s_i) = \deg(s_i)^k$, where $\deg(v)$ denotes the degree of the vertex v in G.

Cao et al. [3] mostly analyzed the special case $k = 1$ and obtained results regarding the maximum and minimum entropy by using certain families of graphs. Also for each $k \geq 1$, Ilic proved that the star S_n is unique tree on n vertices that minimizes I_k for $k \geq 1$ [20]. The second minimum was reported in [10].

In this paper we apply the strong mixing variables (SMV) method for studding the extremal values of graph entropies, in general case. Next we will find the unicyclic and bicyclic graphs that minimize $I_f(G)$ in these classes of graphs, with fix number of vertices.

The paper is organized as follows. In Section 2, some concepts and notations in graph theory, majorization and graph entropy are introduced. In Section 3 we introduce the SMV method and more properties of entropies of graphs. In Section 4 extremal properties of graph entropies have been studied.

2 Preliminaries

2.1 Graph theory

A graph $G = (V(G), E(G))$ is an ordered pair of sets $V(G)$ and $E(G)$, where the elements of set $V(G)$ are called vertices or nodes, and the set $E(G)$ is composed of two-element subsets uv of $V(G)$ named edges. Two vertices u and v are called adjacent to each other if $uv \in E(G)$. Throughout this paper we suppose that any two vertices are connected by at most one edge in G. The degree $\deg(v)$ of a vertex v is defined as the number of vertices to which v is adjacent. A path is a finite sequence of edges that connect a sequence of vertices, such that the end vertex of one edge in the sequence is the start vertex of the next, and in which no vertex appears more than once. A cycle is a path (with at least one edge) whose first and last vertices are the same. A graph is connected if there exists at least one path between every pair of vertices. If connected graph G has exactly n vertices and m edges with $m - n + 1 = 0, 1, 2$, then the graph G is called tree, unicyclic and bicyclic, respectively. The path P_n is a tree of order n with exactly two vertices of degree 1. The star of order n, denoted by S_n, is the tree with $n - 1$ vertices of degree 1. Let $V(G) = \{v_1, v_2, \ldots, v_n\}$ and $d_i = \deg(v_i)$, for $i = 1, \ldots, n$. Then $D(G) = (d_1, d_2, \ldots, d_n)$ is called the degree sequence of G. Without loss of generality, we assume that $d_1 \geq d_2 \geq \ldots \geq d_n$. We use $\Delta = \Delta(G)$ to denote the maximum degree of G. Actually; $\Delta(G) = d_1$.

2.2 Majorization and the degree sequences of graphs

Majorization is an important tool in deriving inequalities in mathematics [21]. We now recall some definitions and results from this theory which will be kept throughout this paper. At first, we consider non-increasing vectors in $\mathbb{R}^n$; that means for any vector $x = (x_1, \ldots, x_n)$ we assume that $x_1 \geq x_2 \geq \ldots \geq x_n$.

Definition 1. *For two vectors $x = (x_1, x_2, \ldots, x_n)$ and $y = (y_1, y_2, \ldots, y_n)$ in $\mathbb{R}^n$,*

$$x \prec y \quad \text{if} \quad \begin{cases} \sum_{i=1}^{k} x_i \leq \sum_{i=1}^{k} y_i, & k = 1, 2, \ldots, n-1; \\ \sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i. & \end{cases}$$

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

Theorem 1. *The inequality*

$$\sum_{i=1}^{n} f(x_i) \leq \sum_{i=1}^{n} f(y_i)$$

holds for all continuous convex functions f if and only if $x \prec y$.

Proof. See [21], Theorem 4.B.1. ■

Remark 1. *Suppose $I \subset R$ is an interval and $f : I \to R$ is a real-value function. If f'' exists and $f''(x) \geq 0$, for each $x \in I$, then f is a convex function.*

Lemma 1. *Let T be a tree with n vertices and $\Delta(T) \leq n-t$, where $1 \leq t \leq n-2$. Then $D(T) \prec (n-t, t, \underbrace{1, \ldots, 1}_{n-2})$.*

Proof. Let $D(T) = (d_1, d_2, \ldots, d_n)$. Then $d_1 = \Delta(T) \leq n-t$ and $\sum_{i=1}^{k} d_i \leq n+k-2$, where $2 \leq k \leq n-1$. Furthermore, $\sum_{i=1}^{n} d_i = 2|E(T)| = 2n-2$. Hence, $D(T) \prec (n-t, t, \underbrace{1, \ldots, 1}_{n-2})$. ■

By a similar argument, one can obtain the following lemmas:

Lemma 2. *Let G be a unicyclic graph with n vertices and $\Delta(G) \leq n-t$. Then $D(G) \prec (n-t, t+1, 2, \underbrace{1, \ldots, 1}_{n-3})$.*

Lemma 3. *Let G be a bicyclic graph with n vertices and $\Delta(G) \leq n-t$. Then $D(G) \prec (n-t, t+2, 2, 2, \underbrace{1, \ldots, 1}_{n-4})$.*

2.3 Graph entropies

The Shannon's entropy of a probability vector $p = (p_1, p_2, \ldots, p_n)$, namely, $1 \geq p_i > 0$ and $\sum_{i=1}^{n} p_i = 1$, is defined as:

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

In mathematics, monotonous functions are functions between ordered sets that preserve or reverses the given order. As we defined in Introduction, monotonous functions from certain sets of associated objects of graphs into positive real numbers are called information functional.

To define the entropy of a graph G, with the set $V(G) = \{v_1, v_2, \ldots, v_n\}$ of vertices, Cao et al. [3] assigned a probability value to each vertex $v_i \in V(G)$ as:

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

where f represents an arbitrary information functional. They obtained the following probability vector

$$(p(v_1), p(v_2), \ldots, p(v_n)).$$

By using the above vector, the entropy of G was defined as:

Definition 2. *Let $G = (V(G), E(G))$ be a connected graph and f be an arbitrary information functional. The entropy of G is defined as*

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

By considering $f(v_i) = \deg(v_i)^k$, where k is an arbitrary real number, Dehmer defined a novel entropy which is based on degree powers of graphs [13]:

$$I_k(G) = -\sum_{i=1}^{n} \frac{d_i^k}{\sum_{j=1}^{n} d_j^k} \log\left(\frac{d_i^k}{\sum_{j=1}^{n} d_j^k}\right) = \log(\sum_{j=1}^{n} d_j^k) - \sum_{i=1}^{n} \frac{d_i^k \log(d_i^k)}{\sum_{j=1}^{n} d_j^k}.$$

3 Graph entropy and regularity

The SMV method (strong mixing variables method) is very useful in proving symmetric inequalities with more than two variables that have either a too complicated or a too long proof. In order to better describe the SMV method, we refer the reader to [8] and [22]. We now apply this method to study the graph entropies.

Lemma 4. *(General mixing variables lemma) Let $(x_1, x_2, \ldots, x_n)$ be an arbitrary real sequence.*

(1) *Choose $i, j \in \{1, 2, \ldots, n\}$, such that $x_i = \min\{x_1, x_2, \ldots, x_n\}$, $x_j = \max\{x_1, x_2, \ldots, x_n\}$.*

(2) *Replace x_i and x_j by it's average $\frac{x_i+x_j}{2}$. (their orders don't change). After infinitely many of the above transformations, each number $x_i, i = 1, 2, \ldots, n,$ tends to the same limit $t = \frac{x_1+x_2+\ldots+x_n}{n}$.*

Proof. See [22]. ∎

Theorem 2. *(SMV theorem) Let $F : I \subseteq R^n \to R$ be a symmetric, continuous, function satisfying $F(a_1, a_2, \dots, a_n) \geq F(b_1, b_2, \dots, b_n)$, where the sequence $(b_1, b_2, \dots, b_n)$ is a sequence obtained from the sequence $(a_1, a_2, \dots, a_n)$ by some predefined transformation (a Ω-transformation). Then we have $F(x_1, x_2, \dots, x_n) \geq F(t, t, \dots, t)$, with $t = \frac{x_1+x_2+\cdots+x_n}{n}$.*

Proof. See [8]. ∎

The transformation Ω can be defined according to the current problem; for example it can be defined as $\frac{a+b}{2}$, $\sqrt{\frac{a^2+b^2}{2}}$, etc.

Theorem 3. *Let $(x_1, x_2, \dots, x_n)$ be a sequence of positive real numbers. Then we have*

$$\ln\left(\sum_{i=1}^{n} x_i\right) - \frac{\sum_{j=1}^{n} x_j \ln(x_j)}{\sum_{k=1}^{n} x_k} \leq \ln(n). \tag{1}$$

Equality occurs iff $x_1 = x_2 = \cdots = x_n$.

Proof. Without loss of generality we may assume that $x_1 \geq x_2 \geq \cdots \geq x_n$. First, let $h(x) = x\ln(x)$. Then $h''(x) = \frac{1}{x} > 0$, and thus h is strictly convex on $(0, +\infty)$. By Jensen's inequality we deduce that

$$h\left(\frac{x_1+x_n}{2}\right) \leq \frac{1}{2}h(x_1) + \frac{1}{2}h(x_n) \quad \Leftrightarrow \quad \left(\frac{x_1+x_n}{2}\right)\ln\left(\frac{x_1+x_n}{2}\right) \leq \frac{1}{2}\ln(x_1) + \frac{1}{2}\ln(x_n), \tag{2}$$

where equality holds if and only if $x_1 = x_n$.

Next, let $g : I \subseteq R^n \to R$ denotes $g(y_1, y_2, \dots, y_n) = \ln(\sum_{i=1}^{n} y_i) - \frac{\sum_{j=1}^{n} y_j \ln(y_j)}{\sum_{k=1}^{n} y_k}$. Then

$$g\left(\frac{x_1+x_n}{2}, x_2, \dots, x_{n-1}, \frac{x_1+x_n}{2}\right) - g(x_1, x_2, \dots, x_n)$$

$$= \frac{-2(\frac{x_1+x_n}{2})\ln(\frac{x_1+x_n}{2}) + x_1\ln(x_1) + x_n\ln(x_n)}{\sum_{i=1}^{n} x_i} \geq 0 \quad \text{by (2)}.$$

Consequently,

$$g\left(\frac{x_1+x_n}{2}, x_2, \dots, x_{n-1}, \frac{x_1+x_n}{2}\right) \geq g(x_1, x_2, \dots, x_n) \tag{3}$$

and equality occurs if and only $x_1 = x_n$. Therefor, by the SMV Theorem, we obtain

$$g(x_1, x_2, \dots, x_n) \leq g(t, t, \dots, t) = \ln(n),$$

where $t = \frac{x_1+x_2+\cdots+x_n}{n}$.

Finally, suppose that $g(x_1, x_2, \dots, x_n) = \ln(n)$ but $x_1 > x_n$. Similar to the above, we see that $\ln(n) \geq g(\frac{x_1+x_n}{2}, x_2, \dots, x_{n-1}, \frac{x_1+x_n}{2})$. Since $x_1 \neq x_n$, (3) shows that

$$\ln(n) \geq g(\frac{x_1+x_n}{2}, x_2, \dots, x_{n-1}, \frac{x_1+x_n}{2}) > g(x_1, x_2, \dots, x_n) = \ln(n),$$

a contradiction. It follows that $x_1 = x_n$. Therefor, $x_1 = x_2 = \cdots = x_n$. ∎

Let us mention three important consequences of Theorem 3.

Corollary 1. *Let G be a connected graph and f be an arbitrary information functional. Then*

$$I_f(G) \leq \ln(n).$$

Equality occurs iff $f(v_i) = f(v_2) = \cdots = f(v_n)$.

Corollary 2. *Let G be a connected graph and $f(v_i) = g(d_i)$. Then*

$$I_f(G) \leq \ln(n).$$

Equality occurs iff $g(d_i) = g(d_2) = \cdots = g(d_n)$. In particular if g is an injective function, the equality holds iff G is a regular graph.

Corollary 3. *Let G be a connected graph and k be a nonzero real number. Then*

$$I_k(G) \leq \ln(n).$$

Equality occurs iff G is a regular graph.

4 Graph entropy of trees, unicyclic and bicyclic graphs

In this section we assume that $D(G) = (d_1, d_2, \ldots, d_n)$ and f is a increasing convex information functional on $D(G)$. Note that every function that is finite and convex on an open interval, is continuous on that interval. Let

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

We give a theorem related to majorization.

Theorem 4. *Let H and G be two non-isomorphic graphs of order n such that $e_{f(H)} \prec e_{f(G)}$. Then $I_f(H) \geq I_f(G)$.*

Proof. Suppose that $D(G) = (d_1(G), \ldots, d_n(G))$ and $D(H) = (d_1(H), \ldots, d_n(H))$. Then

$$\begin{aligned}
e_{f(G)} &= \left(\frac{f(d_1(G))}{\sum_{j=1}^{n} f(d_j(G))}, \frac{f(d_2(G))}{\sum_{j=1}^{n} f(d_j(G))}, \ldots, \frac{f(d_n(G))}{\sum_{j=1}^{n} f(d_j(G))} \right) \\
e_{f(H)} &= \left(\frac{f(d_1(H))}{\sum_{j=1}^{n} f(d_j(H))}, \frac{f(d_2(H))}{\sum_{j=1}^{n} f(d_j(H))}, \ldots, \frac{f(d_n(H))}{\sum_{j=1}^{n} f(d_j(H))} \right)
\end{aligned}$$

Let $h(x) = x\ln(x)$. Then $h''(x) = \frac{1}{x} > 0$, and thus h is convex on $(0,+\infty)$. Since $e_{f(H)} \prec e_{f(G)}$, Theorem 1 shows that

$$\sum_{i=1}^{n} h\left(\frac{f(d_i(H))}{\sum_{j=1}^{n} f(d_j(H))}\right) \le \sum_{i=1}^{n} h\left(\frac{f(d_i(G))}{\sum_{j=1}^{n} f(d_j(G))}\right). \tag{4}$$

But (4) means that $-I_f(H) \le -I_f(G)$. Thus $I_f(H) \ge I_f(G)$, as claimed. ■

Let us mention a simple lemma, which is the key to the main results of this section.

Lemma 5. *Let a, b, c, d be positive integers such that $a \le b$ and $c \le d$. Then*

$$\frac{a}{b} \ge \frac{c}{d} \Leftrightarrow \frac{b-a}{b} \le \frac{d-c}{d}.$$

Proof. The proof is straightforward. ■

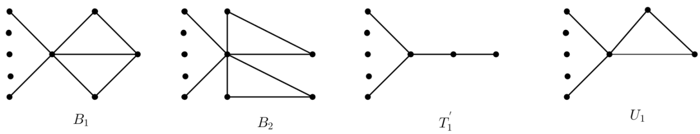

Figure 1. Graphs T_1', B_1, B_2 and U_1.

To characterize the trees, unicyclic and bicyclic graphs that minimize $I_f(G)$ in these classes of graphs, we introduce the graphs T_1', B_1, B_2 and U_1 in Table 1. Fig. 1 illustrates these graphs.

Table 1. Graphs T_1', B_1, B_2 and U_1.

Graph	Degree sequence	Graph	Degree sequence
T_1'	$(n-2, 2, \underbrace{1, \ldots, 1}_{n-2})$	B_1	$(n-1, 3, 2, 2, \underbrace{1, \ldots, 1}_{n-4})$
U_1	$(n-1, 2, 2, \underbrace{1, \ldots, 1}_{n-3})$	B_2	$(n-1, 2, 2, 2, 2, \underbrace{1, \ldots, 1}_{n-5})$

Theorem 5. *Let T be a tree of order n. Then $I_f(T) \ge I_f(S_n)$.*

Proof. We have

$$e_{f(S_n)} = \left(\frac{f(n-1)}{f(n-1)+(n-1)f(1)}, \frac{f(1)}{f(n-1)+(n-1)f(1)}, \ldots, \frac{f(1)}{f(n-1)+(n-1)f(1)}\right).$$

Obviously $\Delta(T) = d_1 \le n-1$. Then by Lemma 1, we have

$$D(T) \prec (n-1, 1, \dots, 1) = D(S_n).$$

Theorem 1 now gives:

$$\sum_{i=1}^{n} f(d_i) \le f(n-1) + (n-1)f(1). \tag{5}$$

Since $\sum_{i=2}^{n} f(d_i) \ge \sum_{i=2}^{n} f(1) = (n-1)f(1)$, (5) shows that

$$\frac{\sum_{i=2}^{n} f(d_i)}{\sum_{j=1}^{n} f(d_j)} \ge \frac{(n-1)f(1)}{f(n-1)+(n-1)f(1)},$$

and

$$\frac{f(d_1)}{\sum_{j=1}^{n} f(d_j)} \le \frac{f(n-1)}{f(n-1)+(n-1)f(1)}, \tag{6}$$

by Lemma 5.

Assume that $i \ge 2$. Then $\frac{f(d_i)}{\sum_{j=1}^{n} f(d_j)} \ge \frac{f(1)}{f(n-1)+(n-1)f(1)}$. Thus, if $n-1 \ge p \ge 2$, then

$$\frac{\sum_{i=p+1}^{n} f(d_i)}{\sum_{j=1}^{n} f(d_j)} = \sum_{i=p+1}^{n} \frac{f(d_i)}{\sum_{j=1}^{n} f(d_j)} \ge \frac{(n-p)f(1)}{f(n-1)+(n-1)f(1)},$$

and by Lemma 5

$$\sum_{i=1}^{p} \frac{f(d_i)}{\sum_{j=1}^{n} f(d_j)} = \frac{\sum_{i=1}^{p} f(d_i)}{\sum_{j=1}^{n} f(d_j)} \le \frac{f(n-1)+(p-1)f(1)}{f(n-1)+(n-1)f(1)}, \quad \text{for } p = 2, \dots, n-1. \tag{7}$$

From $\sum_{i=1}^{n} \frac{f(d_i)}{\sum_{j=1}^{n} f(d_j)} = 1 = \frac{f(n-1)+(n-1)f(1)}{f(n-1)+(n-1)f(1)}$, with (6) and (7) we conclude that $e_f(T) \prec e_f(S_n)$. Applying Theorem 4 to this, we get $I_f(T) \ge I_f(S_n)$. ∎

Theorem 6. *Let $T \ncong S_n$ be a tree of order n. Then $I_f(T) \ge I_f(T_1^{'})$.*

Proof. We have

$$\begin{aligned} e_{f(T_1^{'})} = \Bigg(& \frac{f(n-2)}{f(n-2)+f(2)+(n-2)f(1)}, \frac{f(2)}{f(n-2)+f(2)+(n-2)f(1)}, \\ & \frac{f(1)}{f(n-2)+f(2)+(n-2)f(1)}, \dots, \frac{f(1)}{f(n-2)+f(2)+(n-2)f(1)} \Bigg). \end{aligned}$$

Because $T_1^{'}$ is the unique tree with $\Delta = n-2$ and because $2 \le d_2 \le d_1 = \Delta \le n-2$, Lemma 1 implies that

$$D(T) \prec (n-2, 2, 1, \dots, 1) = D(T_1^{'}).$$

So, by Theorem 1,

$$\sum_{i=1}^{n} f(d_i) \le f(n-2) + f(2) + (n-2)f(1). \tag{8}$$

Since $\sum_{i=2}^{n} f(d_i) \geq f(2) + \sum_{i=3}^{n} f(1) = f(2) + (n-2)f(1)$, (8) shows that

$$\frac{\sum_{i=2}^{n} f(d_i)}{\sum_{j=1}^{n} f(d_j)} \geq \frac{f(2) + (n-2)f(1)}{f(n-2) + f(2) + (n-2)f(1)}.$$

Therefor

$$\frac{f(d_1)}{\sum_{j=1}^{n} f(d_j)} \leq \frac{f(n-2)}{f(n-2) + f(2) + (n-2)f(1)}, \tag{9}$$

by Lemma 5. Similarly, from $\sum_{i=3}^{n} f(d_i) \geq (n-2)f(1)$, (8) and Lemma 5 we conclude that

$$\frac{f(d_1) + f(d_2)}{\sum_{j=1}^{n} f(d_j)} \leq \frac{f(n-2) + f(2)}{f(n-2) + f(2) + (n-2)f(1)}. \tag{10}$$

In addition, for $i \geq 3$, we have $\frac{f(d_i)}{\sum_{j=1}^{n} f(d_j)} \geq \frac{f(1)}{f(n-2)+f(2)+(n-2)f(1)}$. Hence if $n-1 \geq p \geq 3$, then

$$\frac{\sum_{i=p+1}^{n} f(d_i)}{\sum_{j=1}^{n} f(d_j)} \geq \frac{(n-p)f(1)}{f(n-1) + (n-1)f(1)}.$$

Consequently,

$$\sum_{i=1}^{p} \frac{f(d_i)}{\sum_{j=1}^{n} f(d_j)} = \frac{\sum_{i=1}^{p} f(d_i)}{\sum_{j=1}^{n} f(d_j)} \leq \frac{f(n-2) + f(2) + (p-2)f(1)}{f(n-2) + f(2) + (n-2)f(1)}, \quad \text{for } p = 3, \ldots, n-1, \tag{11}$$

by Lemma 5. From $\sum_{i=1}^{n} \frac{f(d_i)}{\sum_{j=1}^{n} f(d_j)} = 1 = \frac{f(n-2)+f(2)+(n-2)f(1)}{f(n-2)+f(2)+(n-2)f(1)}$, (9), (10) and (11) we get $e_f(T) \prec e_f(T_1')$. Now Theorem 4 completes the proof. ■

The above Theorem yields additional results. Here is an example.

Theorem 7. *(See also [10] Theorem 4.5) Let $T \ncong S_n, T_1'$ be a tree of order n and $k \geq 1$. Then $I_k(T) > I_k(T_1') > I_k(S_n)$.*

Theorem 8. *Let G be a unicyclic graph with $n \geq 4$ vertices. Then*

$$I_f(U_1) \leq I_f(G) \leq I_f(C_n).$$

Proof. Let $A_n := f(n-1) + 2f(2) + (n-3)f(1)$. Then we have

$$e_{f(U_1)} = \left(\frac{f(n-1)}{A_n}, \frac{f(2)}{A_n}, \frac{f(2)}{A_n}, \frac{f(1)}{A_n}, \ldots, \frac{f(1)}{A_n} \right).$$

Since C_n is the only regular unicyclic graph, Corollary 1 shows that $I_f(G) \leq \log(n) = I_f(C_n)$. Now suppose that $G \ncong C_n$ and $D(T) = (d_1, d_2, \ldots, d_n)$. Note that G contains a cycle of length at least 3. Thus, $d_1 \geq 3$, $d_2, d_3 \geq 2$ and $d_1 \leq n-1$. Therefore

$$D(G) \prec (n-1, 2, 2, 1, \ldots, 1) = D(U_1),$$

by Lemma 2. So, by Theorem 1, we obtain

$$\sum_{i=1}^{n} f(d_i) \leq f(n-1) + 2f(2) + (n-3)f(1). \qquad (12)$$

Since $\sum_{i=2}^{n} f(d_i) \geq f(2) + f(2) + \sum_{i=4}^{n} f(1) = 2f(2) + (n-3)f(1)$, (12) implies that

$$\frac{\sum_{i=2}^{n} f(d_i)}{\sum_{j=1}^{n} f(d_j)} \geq \frac{2f(2) + (n-3)f(1)}{A_n}.$$

Consequently,

$$\frac{f(d_1)}{\sum_{j=1}^{n} f(d_j)} \leq \frac{f(n-1)}{A_n}, \qquad (13)$$

by Lemma 5. Similarly, we can prove that

$$\frac{f(d_1)+f(d_2)}{\sum_{j=1}^{n} f(d_j)} \leq \frac{f(n-1)+f(2)}{A_n}, \quad \frac{f(d_1)+f(d_2)+f(d_3)}{\sum_{j=1}^{n} f(d_j)} \leq \frac{f(n-1)+2f(2)}{A_n}, \qquad (14)$$

and

$$\sum_{i=1}^{p} \frac{f(d_i)}{\sum_{j=1}^{n} f(d_j)} = \frac{\sum_{i=1}^{p} f(d_i)}{\sum_{j=1}^{n} f(d_j)} \leq \frac{f(n-1)+2f(2)+(p-3)f(1)}{A_n}, \quad \text{for } p = 4, \ldots, n-1.$$

(15)

Now from $\sum_{i=1}^{n} \frac{f(d_i)}{\sum_{j=1}^{n} f(d_j)} = 1 = \frac{f(n-2)+2f(2)+(n-3)f(1)}{A_n}$, (13), (14) and (15) we deduce that $e_f(G) \prec e_f(U_1)$. Hence $I_f(U_1) \leq I_f(G)$, as claimed. ∎

Because $f(x) = x^k$, for $k \geq 1$ is a increasing convex function, we obtain the following important consequence of Theorem 8.

Corollary 4. *Let $G \ncong C_n, U_1$ be a unicyclic graph with $n \geq 4$ vertices and $k \geq 1$. Then*

$$I_k(U_1) < I_k(G) < I_k(C_n).$$

Theorem 9. *Let G be a bicyclic graph with order $n \geq 5$ and $d_2 \geq 3$. Then*

$$I_f(B_1) \leq I_f(G).$$

Proof. It is easy to check that B_1, B_2 are only bicyclic graphs with $\Delta = n-1$. Hence, $d_1 = \Delta(G) \leq n-2$ and by Lemma 3,

$$D(G) \prec (n-1, 3, 2, 2, 1, \ldots, 1) = D(B_1).$$

Therefore, Theorem 1 yields

$$\sum_{i=1}^{n} f(d_i) \leq f(n-1) + f(3) + 2f(2) + (n-4)f(1).$$

Now, by a similar argument applied in Theorem 8, we get $I_f(G) \geq I_f(B_1)$. ∎

An immediate consequence of Theorem 9 is:

Corollary 5. *Let G be a bicyclic graph with order $n \geq 5$ and $d_2 \geq 3$. Then for $k \geq 1$ we have*

$$I_k(B_1) \leq I_k(G).$$

Let T_2 be the tree with $D(T_2) = (3, \underbrace{2, \ldots, 2}_{n-4}, 1, 1, 1)$. Our observation leads to the following conjecture:

Conjecture 1. *Let T be a tree of order n. Then $I_f(T) \leq I_f(P_n)$. If $T \ncong P_n$, then $I_f(T) \leq I_f(T_2)$.*

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References

[1] J. Aczel, Z. Daroczy, *On Measures of Information and Their Characterizations*, Academic Press, New York, 1975.

[2] C. Arndt, *Information Measures*, Springer, Berlin, 2004.

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

[4] S. Cao, M. Dehmer, Z. Kang, Network entropies based on independent sets and matchings, *Appl. Math. Comput.* **307** (2017) 265–270.

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

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

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

[8] Z. Cvetkovski, *Inequalities – Theorems, Techniques and Selected Problems*, Springer, Berlin, 2012, chapter 18.

[9] Z. Daroczy, A. Jarai, On the measurable solutions of functional equation arising in information theory, *Acta Math. Acad. Sci. Hung.* **34** (1979) 105–116.

[10] K. Das, Y. Shi, Some properties on entropies of graphs, *MATCH Commun. Math. Comput. Chem.* **78** (2017) 259–272.

[11] M. Dehmer, A. Mowshowitz, Generalized graph entropies, *Complexity* **17** (2011) 45–50.

[12] M. Dehmer, X. Li, Y. Shi, Connections between generalized graph entropies and graph energy, *Complexity* **21** (2015) 35–41.

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

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

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

[16] M. Dehmer, F. Emmert–Streib, Z. Chen, X. Li, Y. Shi, *Mathematical Foundations and Applications of Graph Entropy*, Wiley, New York, 2016.

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

[18] F. Emmert–Streib, M. Dehmer, Exploring statistical and population aspects of network complexity, *PLoS ONE* **7** (2012) #e34523.

[19] A. Ilić, M. Dehmer, On the distance based graph entropies, *Appl. Math. Comput.* **269** (2015) 647–650.

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

[21] A. W. Marshall, I. Olkin, *Inequalities, Theory of Majorization*, Academic Press, New York, 1979.

[22] T. Puong, *Diamonds in Mathematical Inequalities*, Hanoi Pub. House, 2007.

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

[24] C. E. Shannon, W. Weaver, *The Mathematical Theory of Communication*, Univ. Illinois Press, Urbana, 1949.

[25] C. E. Shannon, A mathematical theory of communication, *Bell. System Tech. J.* **27** (1948) 379–423.

[26] E. Trucco, A note on the information content of graphs, *Bull. Math. Biol.* **18** (1965) 129–135.