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# A Note on Extremality of the First Degree–Based Entropy

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**Abstract**

Let $G$ be a connected graph of order $n$ with degree sequence $D(G) = [d_1, d_2, \ldots, d_n]$. The first degree-based entropy of $G$ is defined as

$$I_1(G) = \ln(\sum_{i=1}^{n} d_i) - \frac{1}{\sum_{i=1}^{n} d_i} \sum_{i=1}^{n} (d_i \ln d_i).$$

In this paper, we characterize the corresponding extremal graphs which attain the maximum value of $I_1(G)$ among all $k$-cyclic graphs of order $n$, where $k \geq 1$.

## 1 Introduction

The information content of graphs and networks have been studied in the last fifties based on the profound and initial works due to Shannon [11, 12]. The concept of graph entropy has been introduced to measure the structural complexity of graphs and networks [10, 13], which is also an information-theoretic quantity that has been introduced by Mowshowitz [9]. Moreover, many graph invariants, such as the number of vertices or edges, the vertex degree sequences, have been used for developing entropy-based measures to characterize the structure of complex network [4–7]. In this paper, we use degree powers to present graph entropies, which has been proven useful in information theory, social network, network reliability and mathematical chemistry [1, 2].

Let $G = (V(G), E(G))$ be a simple connected graph with $n$ vertices and $m$ edges, where $V(G) = \{1, 2, \dots, n\}$ is called the vertex set, and the edge set $E(G)$ is composed of two-element subset $ij$ of $V(G)$ named edges, i.e., $i \sim j$ if $ij \in E(G)$. Let $N_G(i) = \{j \in V(G) \mid j \sim i\}$ be the neighborhood of $i$ and $d_i = |N_G(i)|$ be the degree of $i$. Denote by $D(G) = [d_1, d_2, \dots, d_n]$ the degree sequence of $G$. The cyclomatic number of $G$, written as $k$, is the minimum number of edges we need to remove from the graph such that the resulting graph admits no more cycles. It is well-known that $k = m - n + 1$ and in this situation, $G$ is said to be a $k$-cyclic graph.

Recently, Cao, Dehmer and Shi in [3] introduced the following special degree-based graph entropy by extending the Shannon's entropy:

$$I_s(G) = \ln\left(\sum_{i=1}^{n} d_i^s\right) - \frac{1}{\sum_{i=1}^{n} d_i^s}\sum_{i=1}^{n}(d_i^s \ln d_i^s). \tag{1}$$

The authors mostly analyzed the special case that $G$ is a tree, unicyclic graph, bicyclic graph for $s = 1$. Therefore in this note, we consider $k$-cyclic graphs with $k \geq 1$, which generalizes the main result of Cao et al. [3].

Suppose $s = 1$, observe that

$$\sum_{i=1}^{n} d_i^s = \sum_{i=1}^{n} d_i = 2m.$$

From Equality (1), we infer

$$I_1(G) = \ln\left(\sum_{i=1}^{n} d_i\right) - \frac{1}{\sum_{i=1}^{n} d_i}\sum_{i=1}^{n}(d_i \ln d_i) = \ln(2m) - \frac{1}{2m}\sum_{i=1}^{n}(d_i \ln d_i), \tag{2}$$

which is called the first degree-based entropy of a connected graph by Ghalavand et al. in [8]. Therefore, if we consider the extremal values of $I_1(G)$ of a class of graphs with given number of edges, it suffices to determine the extremal values of $\sum_{i=1}^{n}(d_i \ln d_i)$.

Now we define a function $h(G) = \sum_{i=1}^{n}(d_i \ln d_i)$. In what follows, we consider the extremal values of $h(G)$ for $k$-cyclic graphs, from which we can easily obtain the extremal values of the graph entropy.

Let $G$ be a connected graph with $D(G) = [d_1, d_2, \dots, d_n]$ such that $d_i \geq d_j + 2$ for some pair of $i, j \in V(G)$, then there must exist a vertex $v \in V(G)$ such that $i \sim v$ and $j \nsim v$. Let $G'$ be the graph obtained from $G$ by removing the edge $iv$ and adding the edge $jv$. It is clear that $G'$ has the sequence $[d_1, d_2, \dots, d_i - 1, \dots, d_j + 1, \dots, d_n]$, i.e., by replacing the pair $(d_i, d_j)$ by the pair $(d_i - 1, d_j + 1)$. Obviously, the sum of all degree powers of $G$

equals the sum of all degree powers of $G'$. The next Lemma gives a relationship between the $h(G)$ and $h(G')$.

**Lemma 1.1** (Lemma 1, [3])**.** *For graphs $G$ and $G'$ shown above, we have $h(G) > h(G')$.*

**Proof.** Observe that $d_i > d_i - 1 \geq d_j + 1 > d_j$ since $d_i \geq d_j + 2$. We obtain

$$\begin{aligned} h(G) - h(G') &= d_i \ln d_i + d_j \ln d_j - (d_i - 1)\ln(d_i - 1) - (d_j + 1)\ln(d_j + 1) \\ &= (d_i \ln d_i - (d_i - 1)\ln(d_i - 1)) - ((d_j + 1)\ln(d_j + 1) - d_j \ln d_j) \\ &= (\ln \xi_1 + 1) - (\ln \xi_2 + 1) > 0, \end{aligned}$$

where $\xi_1 \in (d_i - 1, d_i)$ and $\xi_2 \in (d_j, d_j + 1)$. ■

## 2 Extremality of the first degree–based entropy

If $G$ is a connected $k$-cyclic graph of order $n$ having $a_i$ vertices of degree $d_i (i = 1, 2, \ldots, t)$, where $d_1 > d_2 > \cdots > d_t$ and $\sum_{i=1}^{t} a_i = n$, we write the degree sequence of $G$ as $D(G) = [d_1^{a_1}, d_2^{a_2}, \ldots, d_t^{a_t}]$.

- If $2(k-1)$ is divisible by $n$, written as $n | 2(k-1)$, we define a connected $r$-regular $k$-cyclic graph $G_1$ on $n$ vertices such that

$$r = 2 + \frac{2(k-1)}{n}. \tag{3}$$

- If $2(k-1)$ is not divisible by $n$, written as $n \nmid 2(k-1)$, we define a connected $k$-cyclic graph $G_2$ of order $n$ with degree sequence $D(G_2) = [(d+1)^{a_1}, d^{a_2}]$, where

$$\begin{cases} d = \lceil 1 + \frac{2k-2}{n} \rceil, \\ a_1 = (2-d)n + 2k - 2, \\ a_2 = (d-1)n - 2k + 2. \end{cases} \tag{4}$$

Now we aim to study the minimum value of $h(G)$ among all connected $k$-cyclic graphs.

**Lemma 2.1.** *Let $G$ be a connected $k$-cyclic graph of order $n$, where $k \geq 1$ and $G_1, G_2$ be the graphs defined above. Then one of the following two assertions occurs:*

*(i) if $n | 2(k-1)$, it holds that $h(G) \geq h(G_1)$, the equality holds if and only if $G \cong G_1$,*

*(ii) if $n \nmid 2(k-1)$, it holds that $h(G) \geq h(G_2)$, the equality holds if and only if $G \cong G_2$.*

**Proof.** Suppose that $G_{min}$ attains the minimum value of $h(G)$ among all connected $k$-cyclic graphs of order $n$ with $m = k + n - 1$ edges, and $G_{min}$ has the degree sequence $D(G_{min}) = [d_1, d_2, \ldots, d_n]$ satisfying $d_1 \geq d_2 \geq \cdots \geq d_n$. We claim that for each pair of $(d_i, d_j)$, it occurs that

$$d_i = d_j \quad \text{or} \quad d_i = d_j + 1.$$

Otherwise if there exists a pair $(d_i, d_j)$ such that $d_i \geq d_j + 2$, then there must exist a vertex $v$ such that $i \sim v$ and $j \not\sim v$. We construct a $k$-cyclic graph $G'$ obtained from $G_{min}$ by removing the edge $iv$ and adding the edge $jv$, i.e., by replacing the pair $(d_i, d_j)$ by the pair $(d_i - 1, d_j + 1)$. Then by Lemma 1.1, we obtain that $h(G_{min}) > h(G')$, which contradict the minimality of $G_{min}$. In particular, it holds that

$$d_1 = d_n \quad \text{or} \quad d_1 = d_n + 1. \tag{5}$$

Now we partition the discussion into the following two parts.

**Case 1.** $n | 2(k-1)$.

Let $\frac{2(k-1)}{n} = p$, where $p$ is a positive integer. We will show that $d_1 = d_n$, i.e., $G_{min}$ is a regular graph. Otherwise, by Eq. (5), it follows that $d_1 = d_n + 1$. So we can assume that $D(G_{min}) = [(d_n + 1)^{a_1}, d_n^{a_2}]$ with $a_1 > 0, a_2 > 0$. Obviously,

$$\begin{cases} a_1 + a_2 = n, \\ a_1 \cdot (d_n + 1) + a_2 \cdot d_n = 2m = 2(n + k - 1), \end{cases} \tag{6}$$

which gives that

$$\begin{cases} a_1 = (2 - d_n)n + 2(k-1), \\ a_2 = (d_n - 1)n - 2k + 2. \end{cases}$$

Since $a_1 = (2 - d_n)n + 2(k-1) > 0, a_2 = (d_n - 1)n - 2k + 2 > 0$, we obtain that

$$1 + \frac{2(k-1)}{n} < d_n < 2 + \frac{2(k-1)}{n},$$

which is equivalent to

$$1 + p < d_n < 2 + p. \tag{7}$$

Note that $p, d_n$ are all positive integers, which is impossible due to Eq. (7). Therefore $d_1 = d_n$ and $G_{min}$ is a regular graph. Since $nd_n = 2m = 2(k+n-1)$, then $d_n = 2 + \frac{2(k-1)}{n}$. Hence $G_{min} \cong G_1$ .

**Case 2.** $n \nmid 2(k-1)$.

Let $\frac{2(k-1)}{n} = p$, where $p$ is not an integer. We claim that $d_1 = d_n + 1$. Otherwise by Eq. (5), it follows that $d_1 = d_n$, then $nd_n = 2m = 2(k+n-1)$. Hence $d_n = 2 + \frac{2(k-1)}{n} = 2 + p$. Since $p$ is not an integer, then $d_n$ is also not an integer, a contradiction. Hence $d_1 = d_n + 1$ and we assume that $D(G_{min}) = [(d_n+1)^{a_1}, d_n^{a_2}]$ with $a_1 > 0, a_2 > 0$. Similarly, according to Eq. (6) in Case 1, we obtain that

$$1 + \frac{2(k-1)}{n} < d_n < 2 + \frac{2(k-1)}{n}.$$

Therefore $d_n = \lceil 1 + \frac{2(k-1)}{n} \rceil = \lfloor 2 + \frac{2(k-1)}{n} \rfloor$ and

$$\begin{cases} a_1 = (2 - \lceil 1 + \frac{2(k-1)}{n} \rceil)n + 2(k-1), \\ a_2 = (\lceil 1 + \frac{2(k-1)}{n} \rceil - 1)n - 2k + 2, \end{cases}$$

which gives that

$$D(G_{min}) = \left[ \left( \left\lceil 1 + \frac{2(k-1)}{n} \right\rceil + 1 \right)^{(2 - \lceil 1 + \frac{2(k-1)}{n} \rceil)n + 2(k-1)}, \left\lceil 1 + \frac{2(k-1)}{n} \right\rceil^{(\lceil 1 + \frac{2(k-1)}{n} \rceil - 1)n - 2k + 2} \right].$$

Hence $G_{min} \cong G_2$. ∎

Combining Lemma 2.1 with Eq. (2), we finally get the following result towards the extremal properties of the graph entropy.

**Theorem 2.1.** *Let $G$ be a connected $k$-cyclic graph($k \geq 1$) with $n$ vertices. Then one of the following conditions holds:*

*(i) if $n \mid 2(k-1)$, $I_1(G) \leq I_1(G_1)$, the equality holds if and only if $G \cong G_1$,*

*(ii) if $n \nmid 2(k-1)$, $I_1(G) \leq I_1(G_2)$, the equality holds if and only if $G \cong G_2$.*

**Remark 1.** *Let $G$ be a connected $k$-cyclic graph of order $n$ with degree sequence $D(G) = [d_1, d_2, \ldots, d_n]$.*

- *If $n \mid 2(k-1)$ and $G$ is not isomorphic to $G_1$, together with Case 1 in the proof of Lemma 2.1, we observe that $d_1 \neq d_n + 1$. Then we deduce that there exists a pair $(d_i, d_j)$ such that $d_i \geq d_j + 2$. In this situation, there also exists a vertex $v \in V(G)$ satisfying $i \sim v$ and $j \nsim v$. Let $G^*$ be the graph obtained from $G$ by removing the edge $iv$ and adding the edge $jv$. Continue this process until there is no pair $(d_i, d_j)$ such that $d_i \geq d_j + 2$. Thus we obtain a $k$-cyclic graph sequence $G, G^*, G_1^*, \ldots, G_s^*$ such that $G_s^* \cong G_1$.*

- *If $n \nmid 2(k-1)$ and $G$ is not isomorphic to $G_2$, after the same operation as above, we can obtain a graph $G_s^{**}$ such that for each pair $(d_i, d_j)$, it occurs that $d_i = d_j$ or $d_i = d_j + 1$. Combining with Case 2 in the proof of Lemma 2.1, we have $d_1 = d_n + 1$ and $G_s^{**} \cong G_2$.*

Now we consider two particular cases in which $k \in \{1, 2\}$. We conclude this paper by the following two Corollaries, which can be deduced from the result of [3].

**Corollary 2.1** (Theorem 2, [3]). *Let $G$ be a unicyclic graph(1-cyclic graph) of order $n$, then $I_1(G) \leq I_1(C_n)$, where $C_n$ is a cycle of order $n$. The equality holds if and only if $G \cong C_n$.*

**Proof.** By Theorem 2.1, if $k = 1$, then for each unicyclic graph of order $n$, it holds that $n \mid 2(k-1) = 0$. According to Eq. (3), the corresponding extremal graph $G_1$ is a 2-regular unicyclic graph, i.e., $G_1$ is a cycle. ■

**Corollary 2.2** (Theorem 3, [3]). *Let $G$ be a bicyclic graph(2-cyclic graph) of order $n$, then $I_1(G) \leq I_1(G_2)$, where $G_2$ is a connected bicyclic graph with degree sequence $D(G_2) = [3^2, 2^{n-2}]$. The equality holds if and only if $G \cong G_2$.*

**Proof.** By Theorem 2.1, if $k = 2$, then for each bicyclic graph of order $n (n > 2)$, it follows that $n \nmid 2(k-1) = 2$. From Eq. (4), we have $d = 2, a_1 = 2, a_2 = n - 2$. Then the corresponding extremal graph $G_2$ is an irregular graph with degree sequence $D(G_2) = [3^2, 2^{n-2}]$. ■

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