

# First degree-based entropy of graphs

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Received: 6 November 2017

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**Abstract** The first degree-based entropy of a connected graph  $G$  is defined as:  $I_1(G) = \log(\sum_{v_i \in V(G)} \deg(v_i)) - \sum_{v_j \in V(G)} \frac{\deg(v_j) \log \deg(v_j)}{\sum_{v_i \in V(G)} \deg(v_i)}$ . In this paper, we apply majorization technique to extend some known results about the maximum and minimum values of the first degree-based entropy of trees, unicyclic and bicyclic graphs.

**Keywords** Entropy · Tree · Degree sequence · Unicyclic graph · Bicyclic graph

## 1 Introduction

Throughout this paper all graphs are assumed to be simple and undirected and logarithms are in base 2. Suppose  $G$  is such a graph with exactly  $n$  vertices,  $m$  edges and  $k$  connected components. The cyclomatic number of  $G$ ,  $\gamma(G)$ , is the minimum number of edges we need to remove from the graph so that the graph admits no more cycles. It is well-known that  $\gamma(G) = m - n + k$ . If  $k = 1$  and  $\gamma(G) = 0, 1$  or  $2$  then the graph is called tree, unicyclic or bicyclic graph, respectively.

The set of all vertices adjacent to a given vertex  $u$  is denoted by  $N_G(u)$  and such vertices are called neighbors of  $u$ . The number of vertices in  $N_G(u)$ , denoted by  $\deg(u)$ , is the vertex of  $u$  and we use the notations  $\Delta = \Delta(G)$  and  $\delta = \delta(G)$  to denote the maximum and minimum degrees of elements in  $G$ , respectively. The number of

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vertices of degree  $i$  will be denoted by  $n_i(G)$ . It is easy to see that  $\sum_{i=1}^{\Delta(G)} n_i = |V(G)|$ . Suppose that  $V(G) = \{v_1, \dots, v_n\}$  and  $\deg(v_k) = d_k$ , for  $k = 1, \dots, n$ . The sequence  $D(G) = (d_1, d_2, \dots, d_n)$  is called the degree sequence of  $G$ .

For an edge  $uv$  in a graph  $G$ , the subgraph constructed by deleting the edge  $uv$  is denoted by  $G - uv$  and if  $x$  and  $y$  are not adjacent in  $G$ , then  $G + xy$  will be used for graph obtained from  $G$  by adding the edge  $xy$ . The path graph and the star graph with  $n$  vertices are denoted by  $P_n$  and  $S_n$ , respectively. The set of all  $n$ -vertex trees, unicyclic graphs and bicyclic graphs are denoted by  $\tau(n)$ ,  $\mathcal{U}_n$  and  $\mathcal{B}_n$ , respectively.

Complexity as a concept is widely used in various branches of science such as physics, biology, chemistry, mathematics, computer science and economics. To apply complexity in mathematics, measuring complexity is becoming increasingly important. One of the approaches to this propose is the information-theoretic entropy-based measure, which was first introduced by Shannon [19]. In graphs and networks, the concept of graph entropy measure have been initiated based on the important works due to Rashevsky [18] and Trucco [20]. Since there is no unique measure to determine the structural complexity of graphs, up to now a wide range of graph entropy measures have been defined [1, 2, 6, 9]. In addition, several graph invariants, such as the number of vertices, the degree sequences, and the distances between vertices have been used for developing graph entropy measures [3–5, 10–13, 15].

Recently, Chen et al. [4] introduced the following distance-based graph entropy:

**Definition 1.1** Let  $G$  be a simple graph with vertex set  $V(G) = \{v_1, v_2, \dots, v_n\}$ . Then for each positive integer  $k$ ,

$$I_k(G) = \log \sum_{i=1}^n n_k(v_i)^k - \frac{1}{\sum_{i=1}^n n_k(v_i)^k} \sum_{j=1}^n n_k(v_j)^k \log n_k(v_j)^k,$$

where  $n_k(v)$  represents the number of vertices on the distance  $k$  from  $v$ .

If  $k = 1$ , then this is just the same case of the entropy defined based on degree powers by Chen, Dehmer and Shi in [3]. Note that, if  $k = 1$  and  $|E(G)| = m$ , then  $n_k(v) = \deg(v)$  and  $\sum_{i=1}^n n_1(v_i) = 2m$ . Consequently,

$$\begin{aligned} I_1(G) &= \log \sum_{i=1}^n n_1(v_i) - \frac{1}{\sum_{i=1}^n n_1(v_i)} \sum_{i=1}^n n_1(v_i) \log n_1(v_i) \\ &= \log 2m - \frac{1}{2m} \sum_{i=1}^n \deg(v_i) \log \deg(v_i) \\ &= \log 2m - \frac{1}{2m} \sum_{i=1}^n d_i \log d_i. \end{aligned}$$

Therefore, we may assume that  $I_1$  is defined on the degree sequence of  $G$ . In [3], the first maximum and minimum of  $I_1$  for certain families of graphs, namely, trees, unicyclic graphs, bicyclic graphs, chemical trees and chemical graphs, were reported.

In this paper, by using the majorization technique and Schur-convex functions [17], we obtain the other extremal values of  $I_1$ .

We encourage the interested readers to consult the recent book of Dehmer et al. [8] and references therein for more information on graph entropy.

## 2 Preliminary results

Majorization is an important tool in deriving inequalities in mathematics [17]. To proceed further, we first introduce the main concepts and ideas of this method for comparing degree sequences of graphs. For two non-increasing vectors  $d = (d_1, d_2, \dots, d_n)$  and  $d' = (d'_1, d'_2, \dots, d'_n)$  in  $R^n$ , if

$$\sum_{i=1}^k d_i \leq \sum_{i=1}^k d'_i, \quad k = 1, 2, \dots, n-1$$

and

$$\sum_{i=1}^n d_i = \sum_{i=1}^n d'_i,$$

then we say that  $d$  majorizes  $d'$ , written as  $d \leq d'$ . Furthermore,  $d < d'$  means that  $d \leq d'$  and  $d \neq d'$ . A non-increasing sequence  $(d_1, d_2, \dots, d_n)$  of nonnegative integers is said to be graphic if there exists a finite simple graph  $G$  with vertices  $v_1, v_2, \dots, v_n$  such that each  $v_i$  has degree  $d_i$ .

Suppose

$$(d_1, d_2, \dots, d_n) = (\underbrace{x_1, \dots, x_1}_{\alpha_1 \text{ times}}, \underbrace{x_2, \dots, x_2}_{\alpha_2 \text{ times}}, \dots, \underbrace{x_t, \dots, x_t}_{\alpha_t \text{ times}}),$$

where  $d_1 = x_1 > x_2 > \dots > x_t = d_n$  and  $\alpha_1, \dots, \alpha_t$  are positive integers such that  $\alpha_1 + \alpha_2 + \dots + \alpha_t = n$ . We then write  $(d_1, d_2, \dots, d_n) = (x_1^{\alpha_1}, x_2^{\alpha_2}, \dots, x_t^{\alpha_t})$ .

For positive integers  $x_1, \dots, x_m$ , and  $\alpha_1, \dots, \alpha_m$ , let  $T(x_1^{\alpha_1}, \dots, x_m^{\alpha_m})$  be the class of trees with  $\alpha_i$  vertices of the degree  $x_i$ ,  $i = 1, \dots, m$ . Note that this class may be empty. Moreover, by a well-known theorem [14, Lemma 1], there exists a tree in  $T(x_1^{\alpha_1}, \dots, x_m^{\alpha_m})$  if and only if  $\sum_{i=1}^m x_i \alpha_i = 2n - 2$ .

**Lemma 2.1** *Let  $T$  be a tree and  $u$  be a vertex of  $T$  such that  $d_u \geq 3$ . If  $v$  is a pendent vertex in  $T$ , then for each  $y \in N_G(u)$  (not on the path joining  $u$  and  $v$ ) we have  $D(T - uy + yv) < D(T)$ .*

*Proof* Suppose that  $T' = T - uy + yv$ ,  $d_T(u) = x$  and

$$D(T) = (d_1, d_2, \dots, d_i, d_{i+1} = x, d_{i+2}, \dots, d_m, \overbrace{1, \dots, 1}^{n-m}).$$

Then, by definition of  $T'$ , we have

$$D(T') = (d_1, d_2, \dots, d_i, d_{i+1} = x - 1, d_{i+2}, \dots, d_m, 2, \overbrace{1, \dots, 1}^{n-(m+1)}).$$

Note that  $T'$  is a tree, because it is connected with  $n$  vertices and  $n - 1$  edges. Now it is easy to see that:

$$\text{For each } k \ (1 \leq k \leq i), \quad \sum_{j=1}^k d_j(D(T)) = \sum_{j=1}^k d_j(D(T')).$$

$$\text{For each } k \ (i + 1 \leq k \leq m), \quad \sum_{j=1}^k d_j(D(T)) > \sum_{j=1}^k d_j(D(T')).$$

$$\text{For each } k \ (m + 1 \leq k \leq n), \quad \sum_{j=1}^k d_j(D(T)) = \sum_{j=1}^k d_j(D(T')).$$

The above expressions give us the result.  $\square$

**Lemma 2.2** *Let  $T$  be an  $n$ -vertex tree such that  $\Delta(T) \leq n - t$ , where  $1 \leq t \leq n - 2$ . Then,*

$$D(T) \leq (n - t, t, \underbrace{1, \dots, 1}_{n-2}).$$

*Proof* Suppose that  $D(T) = (d_1, d_2, \dots, d_n)$ . Then  $d_1 \leq \Delta(T) \leq n - t$  and  $\sum_{i=1}^k d_i \leq n + k - 2$ , where  $2 \leq k \leq n - 1$ . Since  $\sum_{i=1}^n d_i = 2n - 2$ ,

$$D(T) \leq (n - t, t, \underbrace{1, \dots, 1}_{n-2}),$$

proving the lemma.  $\square$

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

**Lemma 2.3** *Let  $G$  be a unicyclic graph with  $n$  vertices and  $\Delta(G) \leq n - t$ . Then,*

$$D(G) \leq (n - t, t + 1, 2, \underbrace{1, \dots, 1}_{n-3}).$$

**Lemma 2.4** *Let  $G$  be a bicyclic graph with  $n$  vertices and  $\Delta(G) \leq n - t$ . Then,*

$$D(G) \leq (n - t, t + 2, 2, 2, \underbrace{1, \dots, 1}_{n-4}).$$

**Theorem 2.5** Let  $G$  and  $G'$  be two connected graphs with non-increasing degree sequences  $D(G) = (d_1, d_2, \dots, d_n)$  and  $D(G') = (d'_1, d'_2, \dots, d'_n)$ .

If  $D(G') \leq D(G)$ , then  $I_1(G') \geq I_1(G)$ , where equality holds if and only if  $D(G') = D(G)$ .

*Proof* Suppose that  $h(G) = \sum_{i=1}^n (d_i \log d_i)$ . Observe that  $d_i \log d_i$  is a strictly convex function; hence,  $h$  is a strictly Schur-convex function. Therefore,  $h(G) \geq h(G')$ , and the equality holds if and only if  $D(G) = D(G')$ . In addition,  $D(G') \leq D(G)$  implies that  $|E(G)| = \sum_{i=1}^n d_i = \sum_{i=1}^n d'_i = |E(G')|$ . Hence  $I_1(G') \geq I_1(G)$ , and the equality holds if and only if  $D(G) = D(G')$ .  $\square$

### 3 Extremal values of $I_1(G)$

Lić [16], proved that the path is the unique tree on  $n$  vertices that maximizes  $I_k(T)$ , for  $k > 0$ , and the star is the unique tree on  $n$  vertices that minimizes  $I_k(T)$ , for  $k \geq 1$ . Das and Shi [7], applied majorization theory to characterize the trees with the second minimum value of  $I_k(T)$ , for  $k \geq 1$ . In this section, we continue this study to obtain the extremal values of  $I_1$  for certain classes of graphs. The following simple lemma will be used later.

**Lemma 3.1** For each  $T \in \tau(n)$ ,

$$n_1(T) = 2 + \sum_{i=3}^{\Delta(T)} n_i(i-2), \quad n_2(T) = n - 2 - \sum_{i=3}^{\Delta(T)} n_i(i-1).$$

*Proof* We have  $n_1 + n_2 + \sum_{i=3}^{\Delta(T)} n_i = n$  and  $n_1 + 2n_2 + \sum_{i=3}^{\Delta(T)} n_i i = 2(n-1)$ . These equations give us the result.  $\square$

**Theorem 3.2** Let  $T$  be a tree with  $n \geq 12$  vertices and  $\Delta(T) = 3$ , such that  $n_3(T) \geq 6$ . Then, for each  $T' \in T(3^5, 2^{n-12}, 1^7)$ , we have  $I_1(T') > I_1(T)$ .

*Proof* The proof is by induction on  $n_3(T)$ . If  $n_3(T) = 6$ , then by applying Lemma 2.1 on a vertex of degree 3 in  $T$ , we obtain a tree, say  $T'$ , with 5 vertices of degree 3. Since  $\Delta(T') = 3$ , Lemma 3.1 proves that  $n_1(T') = 7$  and  $n_2(T') = n - 12$ . Therefore,  $T' \in T(3^5, 2^{n-12}, 1^7)$  and by Lemma 2.1,  $D(T') < D(T)$ . Now Theorem 2.5 gives  $I_1(T') > I_1(T)$ .

Next we assume that  $n_3(T) > 6$ . Again apply Lemma 2.1 to decrease the number of vertices of degree 3. The proof is now deduced from the induction hypothesis.  $\square$

**Theorem 3.3** Let  $T$  be a tree with  $n \geq 12$  vertices and  $\Delta(T) = 4$ . If  $n_4(T) = 1$  and  $n_3(T) \geq 3$ , then for each  $T' \in T(4^1, 3^2, 2^{n-9}, 1^6)$  we have  $I_1(T') > I_1(T)$ .

*Proof* The proof is by induction on  $n_3(T)$ . If  $n_3(T) = 3$ , then by using Lemma 2.1 on a vertex of degree 3 in  $T$ , we obtain a tree, say  $T'$ , with two vertices of degree 3. Since  $\Delta(T') = 4$  and  $n_4(T') = 1$ , Lemma 3.1 proves that  $n_1(T') = 6$  and  $n_2(T') = n - 9$ .

Therefore,  $T' \in T(4^1, 3^2, 2^{n-9}, 1^6)$  and by Lemma 2.1 and Theorem 2.5 we have  $I_1(T') > D(T)$ .

Suppose  $n_3(T) > 3$ . Apply again Lemma 2.1 to decrease the number of vertices of degree 3. The proof now follows from induction hypothesis.  $\square$

**Theorem 3.4** *Let  $T$  be a tree with  $n \geq 12$  vertices and  $\Delta(T) = 4$ . If  $n_4(T) \geq 2$  and  $T \notin T(4^2, 2^{n-8}, 1^6)$ , then for each  $T' \in T(4^2, 2^{n-8}, 1^6)$  we have  $I_1(T') > I_1(T)$ .*

*Proof* By repeated applications of Lemma 2.1 on vertices of degree 4 in  $T$ , for a sufficient number of times ( $t$ -times), we arrive at a tree  $T_t$ , with  $n_4(T_t) = 2$ . Furthermore, by repeated applications of Lemma 2.1 on vertices of degree 3 in  $T_t$ , again for a sufficient number of times ( $s$ -times), we arrive at a tree  $T_s$ , with  $n_4(T_s) = 2$  and  $n_3(T_s) = 0$ . In addition, by Lemma 3.1 we have  $n_1(T_s) = 6$  and  $n_2(T_s) = n - 8$ . Therefore,  $T_s \in T(4^2, 2^{n-8}, 1^6)$  and by Lemma 2.1,  $D(T') = D(T_s) < D(T)$ . The proof now follows from Theorem 2.5.  $\square$

**Theorem 3.5** *Let  $T$  be a tree with  $n(\geq 12)$  vertices and  $\Delta(T) \geq 5$ . If  $T \notin T(5^1, 2^{n-6}, 1^5)$ , then for each  $T' \in T(5^1, 2^{n-6}, 1^5)$  we have  $I_1(T') > I_1(T)$ .*

*Proof* Suppose  $v_1 \in V(T)$ ,  $d_T(v_1) = \Delta(T)$  and set  $U = \{v \in V(T) \mid v \neq v_1, d_T(v) \geq 3\}$ . By repeated applications of Lemma 2.1 on vertices in  $U$  for a sufficient number of times, we arrive at a tree  $T_m$ , with only one vertex  $v_1$  of degree  $\Delta(T)$  and the degree of other vertices is 1 or 2. In addition, by repeated applications of Lemma 2.1 on  $v_1$  for a  $(\Delta(T) - 5)$ -times, we arrive at a tree  $T$ , such that  $n_5(T') = 1$  and  $n_i = 0$ , for  $i \geq 3$  and  $i \neq 5$ . On the other hand, by Lemma 3.1 we have  $n_1(T') = 5$  and  $n_2(T') = n - 6$ . Therefore,  $T' \in T(5^1, 2^{n-6}, 1^5)$  and by Lemma 2.1,  $D(T') < D(T)$ . The proof is now a consequence of Theorem 2.5.  $\square$

**Remark 3.6** For  $n \geq 12$ , let  $T_1 := P_n$ ,  $T_2 \in T(3^1, 2^{n-4}, 1^3)$ ,  $T_3 \in T(3^2, 2^{n-6}, 1^4)$ ,  $T_4 \in T(4^1, 2^{n-5}, 1^4)$ ,  $T_5 \in T(3^3, 2^{n-8}, 1^5)$ ,  $T_6 \in T(4^1, 3^1, 2^{n-7}, 1^5)$ ,  $T_7 \in T(3^4, 2^{n-10}, 1^6)$ ,  $T_8 \in T(4^1, 3^2, 2^{n-9}, 1^6)$ ,  $T_9 \in T(5^1, 2^{n-6}, 1^5)$ ,  $T_{10} \in T(3^5, 2^{n-12}, 1^7)$  and  $T_{11} \in T(4^2, 2^{n-8}, 1^6)$ .

**Theorem 3.7**  $I_1(T_1) > I_1(T_2) > I_1(T_3) > I_1(T_4) > I_1(T_5) > I_1(T_6) > I_1(T_7) > I_1(T_8) > I_1(T_9) > I_1(T_{10}) > I_1(T_{11})$ .

*Proof* Apply Table 1.  $\square$

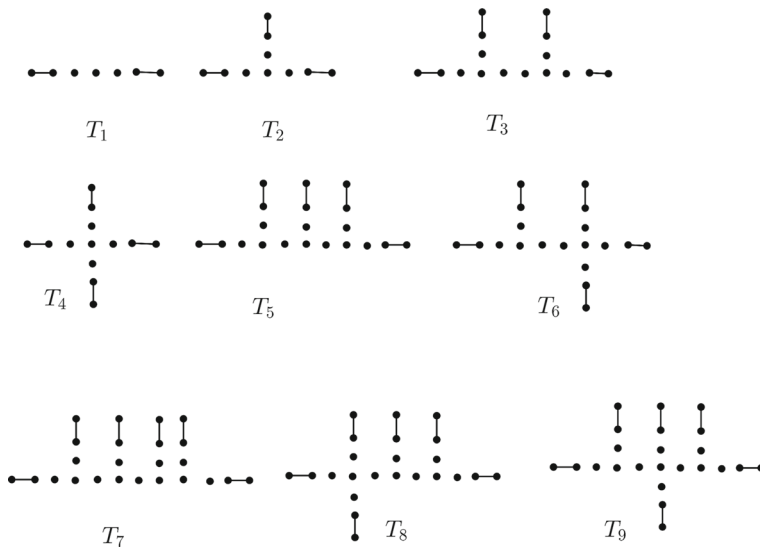
In [3], the authors proved that if  $T$  is a tree with  $n$  vertices, then  $I_1(T) \leq I_1(P_n)$  and the equality holds if and only if  $T = P_n$ . Furthermore,  $I_1(T) \geq I_1(S_n)$  and the equality holds if and only if  $T = S_n$ . We extend these results as follows:

**Theorem 3.8** *If  $n \geq 12$  and  $T \in \tau(n) \setminus \{T_1, T_2, \dots, T_8\}$ , then  $I_1(T_1) > I_1(T_2) > I_1(T_3) > I_1(T_4) > I_1(T_5) > I_1(T_6) > I_1(T_7) > I_1(T_8) > I_1(T)$ .*

*Proof* By Theorem 3.7,  $I_1(T_1) > I_1(T_2) > I_1(T_3) > I_1(T_4) > I_1(T_5) > I_1(T_6) > I_1(T_7) > I_1(T_8)$ . If  $T \in \{T_9, T_{10}, T_{11}\}$ , then the proof follows from Theorem 3.7. If  $\Delta(T) = 3$  and  $n_3(T) \geq 6$ , then by Theorem 3.2 we have  $I_1(T_{10}) > I_1(T)$ . Now Theorem 3.7 gives us the result. Suppose that  $\Delta(T) = 4$ . If  $n_4(T) = 1$  and  $n_3(T) \geq 3$ ,

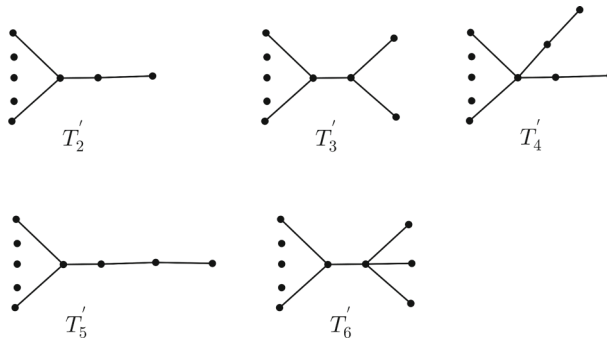
**Table 1** Classes of trees with  $n$  vertices and their entropies

	Class	Values of $I_1$
1	$T(2^{n-2}, 1^2)$	$\log 2m - \frac{1}{2m}((n-12)\log 4 + \log(1048576))$
2	$T(3^1, 2^{n-4}, 1^3)$	$\log 2m - \frac{1}{2m}((n-12)\log 4 + \log(1769472))$
3	$T(3^2, 2^{n-6}, 1^4)$	$\log 2m - \frac{1}{2m}((n-12)\log 4 + \log(2985984))$
4	$T(3^3, 2^{n-8}, 1^5)$	$\log 2m - \frac{1}{2m}((n-12)\log 4 + \log(5038848))$
5	$T(3^4, 2^{n-10}, 1^6)$	$\log 2m - \frac{1}{2m}((n-12)\log 4 + \log(8503056))$
6	$T(3^5, 2^{n-12}, 1^7)$	$\log 2m - \frac{1}{2m}((n-12)\log 4 + \log(14348907))$
7	$T(4^1, 2^{n-5}, 1^4)$	$\log 2m - \frac{1}{2m}((n-12)\log 4 + \log(4194304))$
8	$T(4^1, 3^1, 2^{n-7}, 1^5)$	$\log 2m - \frac{1}{2m}((n-12)\log 4 + \log(7077888))$
9	$T(4^1, 3^2, 2^{n-9}, 1^6)$	$\log 2m - \frac{1}{2m}((n-12)\log 4 + \log(11943936))$
10	$T(4^2, 2^{n-8}, 1^6)$	$\log 2m - \frac{1}{2m}((n-12)\log 4 + \log(16777216))$
11	$T(5^1, 2^{n-6}, 1^5)$	$\log 2m - \frac{1}{2m}((n-12)\log 4 + \log(12800000))$


**Fig. 1** The trees  $T_1, T_2, \dots, T_8$  in Theorem 3.8

then by Theorem 3.3 we have  $I_1(T_8) > I_1(T)$  and the result is a consequence of Theorem 3.7. For the case that  $n_4(T) \geq 2$ , we apply Theorem 3.4 to prove that  $I_1(T_{11}) > I_1(T)$ . Then the result is a consequence of Theorem 3.7. If  $\Delta(T) \geq 5$ , then by Theorem 3.5,  $I_1(T_9) > I_1(T)$  and again Theorem 3.7 gives us the result. Otherwise,  $T \in \{T_1, T_2, \dots, T_8\}$ .  $\square$

**Remark 3.9** Let  $T'_1 := S_n$ ,  $T'_2 \in T((n-2)^1, 2^1, 1^{n-2})$ ,  $T'_3 \in T((n-3)^1, 3^1, 1^{(n-2)})$ ,  $T'_4 \in T((n-3)^1, 2^2, 1^{n-3})$  and  $T'_5 \in T((n-4)^1, 4^1, 1^{n-2})$ ,  $n \geq 10$ . See Fig. 1.

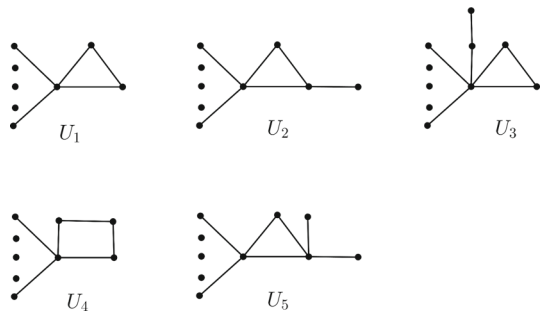


**Fig. 2** The trees  $T'_2, \dots, T'_6$

**Table 2** Some classes of trees and their entropies, see Theorem 3.10

	Class	Values of $I_1$
1	$T((n-1)^1, 1^{n-1})$	$\log 2m - \frac{1}{2m}(n-1) \log(n-1)$
2	$T((n-2)^1, 2^1, 1^{n-2})$	$\log 2m - \frac{1}{2m}((n-2) \log(n-2) + \log(4))$
3	$T((n-3)^1, 3^1, 1^{n-2})$	$\log 2m - \frac{1}{2m}((n-3) \log(n-3) + \log(27))$
4	$T((n-3)^1, 2^2, 1^{n-3})$	$\log 2m - \frac{1}{2m}((n-3) \log(n-3) + \log(16))$
5	$T((n-4)^1, 4^1, 1^{n-2})$	$\log 2m - \frac{1}{2m}((n-4) \log(n-4) + \log(256))$

**Fig. 3** The unicyclic graphs  $U_1, \dots, U_5$



**Theorem 3.10** If  $n \geq 10$  and  $T \in \tau(n) \setminus \{T'_1, T'_2, \dots, T'_5\}$ , then  $I_1(T'_1) < I_1(T'_2) < I_1(T'_3) < I_1(T'_4) = I_1(T'_5) < I_1(T'_6) < I_1(T)$ . See Fig. 2.

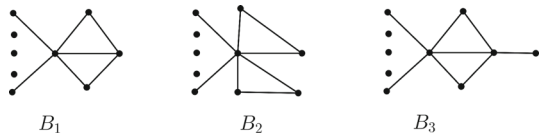
*Proof* By Table 2,  $I_1(S_n) < I_1(T'_2) < I_1(T'_3) < I_1(T'_4) = I_1(T'_5) < I_1(T'_6)$ . Since  $S_n, T'_1, T'_2, \dots, T'_5$  are all trees with  $\Delta \geq n-3$ , if  $T \in \tau(n) \setminus \{S_n, T'_2, \dots, T'_5\}$  then  $\Delta(T) \leq n-4$ . Therefore, by Lemma 2.2 and Theorem 2.5 we have  $I_1(T'_6) < I_1(T)$ .  $\square$

**Theorem 3.11** Let  $n \geq 9$  and  $G \in \mathcal{U}_n \setminus \{U_1, U_2, \dots, U_5\}$ . Then  $I_1(U_1) < I_1(U_2) < I_1(U_3) = I_1(U_4) < I_1(U_5) < I_1(G)$ . See Fig. 3.



**Table 3** Unicyclic graphs in Theorem 3.11 and their entropies ( $m = n$ )

Graph	Degree sequence	Values of $I_1$
$U_1$	$(n - 1, 2, 2, 1, \dots, 1)$	$\log 2m - \frac{1}{2m}((n - 1) \log(n - 1) + \log(16))$
$U_2$	$(n - 2, 3, 2, 1, \dots, 1)$	$\log 2m - \frac{1}{2m}((n - 2) \log(n - 2) + \log(108))$
$U_3$	$(n - 2, 2, 2, 2, 1, \dots, 1)$	$\log 2m - \frac{1}{2m}((n - 2) \log(n - 2) + \log(64))$
$U_4$	$(n - 2, 2, 2, 2, 1, \dots, 1)$	$\log 2m - \frac{1}{2m}((n - 2) \log(n - 2) + \log(64))$
$U_5$	$(n - 3, 4, 2, 1, \dots, 1)$	$\log 2m - \frac{1}{2m}((n - 3) \log(n - 3) + \log(1024))$

**Fig. 4** The bicyclic graphs  $B_1$ ,  $B_2$  and  $B_3$ 

**Table 4** Bicyclic graphs in Theorem 3.12 and their entropy ( $m = n + 1$ )

Graph	Degree sequence	Values of $I_1$
$B_1$	$(n - 1, 3, 2, 2, 1, \dots, 1)$	$\log 2m - \frac{1}{2m}((n - 1) \log(n - 1) + \log(432))$
$B_2$	$(n - 1, 2, 2, 2, 2, 1, \dots, 1)$	$\log 2m - \frac{1}{2m}((n - 1) \log(n - 1) + \log(256))$
$B_3$	$(n - 2, 4, 2, 2, 1, \dots, 1)$	$\log 2m - \frac{1}{2m}((n - 2) \log(n - 2) + \log(4096))$

*Proof* By Table 3,  $I_1(U_1) < I_1(U_2) < I_2(U_3) = I_1(U_4) < I_1(U_5)$ . Also  $U_1, U_2, U_3, U_4$  are all unicyclic graphs with  $\Delta \geq n - 2$ . Therefore, if  $G \in \mathcal{U}_n \setminus \{U_1, U_2, U_3, U_4\}$ , then  $\Delta(G) \leq n - 3$ , and Lemma 2.3 and Theorem 2.5 show that  $I_1(U_5) < I_1(G)$ .  $\square$

**Theorem 3.12** Let  $G \in \mathcal{B}_n \setminus \{B_1, B_2, B_3\}$ , where  $n \geq 8$ . Then  $I_1(B_1) < I_1(B_2) < I_1(B_3) < I_1(G)$ . See Fig. 4.

*Proof* By Table 4,  $I_1(B_1) < I_1(B_2) < I_1(B_3)$ . On the other hand,  $B_1$  and  $B_2$  are bicyclic graphs with  $\Delta \geq n - 1$ . Therefore, if  $G \in \mathcal{B}_n \setminus \{B_1, B_2\}$ , then  $\Delta(G) \leq n - 2$ , and by Lemma 2.4 and Theorem 2.5 we have  $I_1(B_3) < I_1(G)$ .  $\square$

## 4 Concluding remarks

In this paper, we have studied the graph entropy  $I_1(G)$ , for a connected graph  $G$ . Set  $A := \{T_1, T_2, \dots, T_8, T'_1, \dots, T'_6\}$ . By applying majorization theory, it is proved that if  $T \in \tau(n) \setminus A$ , then  $I_1(T'_1) < I_1(T'_2) < I_1(T'_3) < I_1(T'_4) = I_1(T'_5) < I_1(T'_6) < I_1(T)$ . On the other hand,  $I_1(T_1) > I_1(T_2) > \dots > I_1(T_8) > I_1(T)$ . Note that  $T_1, T_2, \dots, T_8$  are chemical trees. Therefore, the last equalities holds for all chemical trees with  $n$  vertices.

**Acknowledgements** We are indebted to the referees for his/her suggestions and helpful remarks led us to improve this paper. The research of the third author is partially supported by the University of Kashan under Grant No. 572760/245.

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