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Extremality of degree-based graph entropies

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ABSTRACT

Many graph invariants have been used for the construction of entropy-based measures to characterize the structure of complex networks. Based on Shannon's entropy, we study graph entropies which are based on vertex degrees by using so-called information functionals. When considering Shannon entropy-based graph measures, there has been very little work to find their extremal values. The main contribution of this paper is to prove some extremal values for the underlying graph entropy of certain families of graphs and to find the connection between the graph entropy and the sum of degree powers. Further, conjectures to determine extremal values of graph entropies are given.

1. Introduction

Studies of the information content of graphs and networks have been initiated in the late fifties based on the seminal work due to Shannon [70]. The concept of graph entropy [20,24] introduced by Rashevsky [67] and Trucco [76] has been used to measure the structural complexity of graphs [11,21,22]. The entropy of a graph is an information-theoretic quantity that has been introduced by Mowshowitz [58]. Here the complexity of a graph [25] is based on the well-known Shannon's entropy [18,20,70,58]. Importantly, Mowshowitz interpreted his graph entropy measure as the structural information content of a graph and demonstrated that this quantity satisfies important properties when using product graphs, etc., see, e.g., [58–61]. Note the Körner's graph entropy [52] has been introduced from an information theory point of view and has not been used to characterize graphs quantitatively. An extensive overview on graph entropy measures can be found in [24]. A statistical analysis of topological graph measures has been performed by Emmert-Streib and Dehmer [29].

Several graph invariants, such as the number of vertices, the vertex degree sequences, extended degree sequences (i.e., the second neighbor, third neighbor, etc.), edges, and connections, have been used for developing entropy-based measures [20,24]. In this paper, we introduce a novel graph entropy, which is based on a new information functional by using degree powers. Degree powers is one of the most important graph invariants, which has been proven useful in information theory, social networks, network reliability and mathematical chemistry, see [9,10]. In view of the vast of amount of existing graph entropy measures [11,20], there has been very little work to find their extremal values [23]. A reason for this might be the fact that Shannon's entropy represents a multivariate function and all probability values are not equal to zero when considering graph entropies. Inspired by Dehmer and Kraus [23], it turned out that determining minimal values of graph entropies

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is intricate because there is a lack of analytical methods to tackle this particular problem. Other related work is due to Shi [71], who proved a lower bound of quantum decision tree complexity by using Shannon's entropy. Dragomir and Goh [28] obtained several general upper bounds for Shannon's entropy by using Jensen's inequality [43]. Finally, Dehmer and Kraus [23] proved some extremal results for graph entropies which are based on information functionals.

The main contribution of the paper is to study novel properties of graph entropies which are based on an information functional by using degree powers of graphs. In particular, we determine the extremal values for the underlying graph entropy of certain families of graphs and find the connection between graph entropy and the sum of degree powers, which is well-studied in graph theory and some related disciplines. Further, conjectures to determine extremal values of graph entropies are proposed.

The paper is organized as follows. In Section 2, some concepts and notation in graph theory are introduced. In Section 3, we introduce some results on the sum of degree powers. In Section 4, we state the definitions of graph entropies based on the given information functional by using degree powers. In Sections 5 and 6, extremal properties of graph entropies have been studied. Further, we express some conjectures to find extremal values of trees. We discuss some potential applications of degree-based entropies in Section 7. The paper finishes with a summary and conclusion in Section 8.

2. Preliminaries

A *graph* G is an ordered pair of sets $V(G)$ and $E(G)$ such that the elements $uv \in E(G)$ are a sub-collection of the unordered pairs of elements of $V(G)$. For convenience, we denote a graph by $G = (V, E)$ sometimes. The elements of $V(G)$ are called *vertices* and the elements of $E(G)$ are called *edges*. If $e = uv$ is an edge, then we say vertices u and v are *adjacent*, and $u,\ v$ are two endpoints (or ends) of e. A *loop* is an edge whose two endpoints are the some one. Two edges are called *parallel*, if both edges have the same endpoints. A *simple graph* is a graph containing no loops and parallel edges. If G is a graph with n vertices and m edges, then we say the *order* of G is n and the *size* of G is m. A graph of order n is addressed as an *n-vertex graph*, and a graph of order n and size m is addressed as an *(n,m)-graph*. A graph F is called a *subgraph* of a graph G, if $V(F) \subseteq V(G)$ and $E(F) \subseteq E(G)$, denoted by $F \subseteq G$. In this paper, we only consider simple graphs.

Let $G = (V(G), E(G))$ and $H = (V(H), E(H))$ be two simple graphs. A *graph isomorphism* from G to H is a bijection $f:\ V(G) \to V(H)$ such that $uv \in E(G)$ if and only if $f(u)f(v) \in E(H)$. If there is a graph isomorphism from G to H, then G is said to be *isomorphic* to H, denoted by $G \cong H$.

A graph is *connected* if, for every partition of its vertex set into two nonempty sets X and Y, there is an edge with one end in X and one end in Y. Otherwise, the graph is *disconnected*. In other words, a graph is *disconnected* if its vertex set can be partitioned into two nonempty subsets X and Y so that no edge has one end in X and one end in Y.

A *path graph* is a simple graph whose vertices can be arranged in a linear sequence in such a way that two vertices are adjacent if they are consecutive in the sequence, and are nonadjacent otherwise. Likewise, a *cycle graph* on three or more vertices is a simple graph whose vertices can be arranged in a cyclic sequence in such a way that two vertices are adjacent if they are consecutive in the sequence, and are nonadjacent otherwise. Denote by P_n and C_n the path graph and the cycle graph with n vertices, respectively.

A connected graph without any cycle is a *tree*. Actually, the path P_n is a tree of order n with exactly two pendent vertices. The *star* of order n, denoted by S_n, is the tree with $n-1$ pendent vertices. A simple connected graph is called *unicyclic* if it has exactly one cycle. We use S_n^+ to denote the unicyclic graph obtained from the star S_n by adding to it an edge between two pendent vertices of S_n. Observe that a tree and a unicyclic graph of order n have exactly $n-1$ and n edges, respectively. A *bicyclic graph* is a graph of order n with $n+1$ edges.

The *length* of a path is the number of its edges. For two vertices u and v, the *distance* between u and v in a graph G, denoted by $d_G(u, v)$, is the length of the shortest path connecting u and v. The *diameter* of a graph G is the greatest distance between two vertices of G.

All vertices adjacent to vertex u are called *neighbors* of u. The *neighborhood* of u is the set of the neighbors of u. The number of edges adjacent to vertex u is the *degree* of u, denoted by $d(u)$. Vertices of degrees 0 and 1 are said to be *isolated* and *pendent vertices*, respectively. A pendent vertex is also referred to as a *leaf* of the underlying graph. A vertex of degree i is also addressed as an *i-degree vertex*. The minimum and maximum degree of G is denoted by $\delta(G)$ and $\Delta(G)$, respectively. If G has a_i vertices of degree d_i $(i = 1, 2, \ldots, t)$, where $\Delta(G) = d_1 > d_2 > \cdots > d_t = \delta(G)$ and $\sum_{i=1}^{t} a_i = n$, we define the *degree sequence* of G as $D(G) = [d_1^{a_1}, d_2^{a_2}, \ldots, d_t^{a_t}]$. If $a_i = 1$, we use d_i instead of $d_i^{a_i}$ for convenience.

In chemical graph theory, a *chemical graph* or *molecular graph* is a representation of the structural formula of a chemical compound in terms of graph theory. Here, a graph corresponds to a chemical structural formula, in which a vertex and an edge correspond to an atom and a chemical bond, respectively. Since carbon atoms are 4-valent, we obtain graphs in which no vertex has degree greater than four. Analogously, a *chemical tree* is a tree T with maximum degree at most four. For a more thorough introduction on chemical graphs, we refer to [12,77].

Let G be a graph of order n. The *adjacency matrix* of a graph G is the $n \times n$ matrix $A(G) := (a_{uv})$, where a_{uv} is the number of edges joining vertices u and v, each loop counting as two edges. If G is simple, then $A(G)$ is a $(0,1)$-matrix. The *eigenvalues* of G is the eigenvalues of its adjacency matrix $A(G)$. All eigenvalues of G forms the spectrum of G, which is widely studied in algebraic graph theory. For this topic, we refer to [34].

For a given graph H, denote by $ex(n,H)$ the classical Turán number, i.e., the largest number of edges among all graphs of order n which do not contain H as a subgraph. The value of $ex(n,H)$ are well-studied in extremal graph theory. For more results, we refer to [7,72].

For terminology and notations not defined here, we refer the readers to [14].

3. Degree powers of graphs

The vertex degree is an important graph invariant, which is related to many properties of graphs. Let G be a graph of order n with degree sequence $d_1, d_2, \ldots, d_n$. The sum of degree powers of a graph G is defined by

$$\sum_{i=1}^{n} d_i^k,$$

where k is an arbitrary real number. Observe that if $k = 1$, then the number is exactly two times of the number of edges. As a graph invariant, the sum of degree powers has received considerable attention in graph theory and extremal graph theory, which is related to the famous Ramsey problems [35,36]. Actually, the sum of degree powers also has many applications in information theory, social networks, network reliability and mathematical chemistry.

The main challenges when dealing with the sum of degree powers are as follows: Let $\mathcal{G}(n,m)$ be the set of all simple graphs with n vertices and m edges.

- What is the maximum or minimum value of $\sum_{i=1}^{n} d_i^k$, for a graph $G \in \mathcal{G}(n,m)$?
- Which graphs $G \in \mathcal{G}(n,m)$ can attain the maximum or the minimum value of $\sum_{i=1}^{n} d_i^k$?

To solve these problems, maximizing the sum of the squares of degrees, i.e., $\sum_{i=1}^{n} d_i^2$, has been firstly performed by Katz [48] in 1971 and by Ahlswede and Katona [2] in 1978. In his review of [2], Erdös [30] commented that "the solution is more difficult than one would expect". Ahlswede and Katona were interested in an equivalent form of the problem. That means, they tried to find the maximum number of pairs of different edges that have a common vertex. In other words, they aim to maximize the number of edges in the line graph $L(G)$ as G ranges over $\mathcal{G}(n,m)$. Ahlswede and Katona showed that the maximum value is always attained at one or both of two special graphs in $\mathcal{G}(n,m)$. On the other hand, Katz's problem was to maximize the sum of the elements in A^2, where A runs over all $(0,1)$-square matrices of size n with precisely j ones. He found the maxima and the matrices for which the maxima are attained for the special cases where there are k^2 ones or where there are $n^2 - k^2$ ones in the $(0,1)$-matrix.

The following Ramsey-type problem was studied by Goodman in [35,36]: Maximize the number of monochromatic triangles in a two-coloring of the complete graph with a fixed number of vertices and a fixed number of red edges. Olpp [63] showed that Goodman's problem is equivalent to finding the two-coloring that maximizes the sum of squares of the red-degrees of the vertices. Of course, a two-coloring of the complete graph on n vertices gives rise to two graphs on n vertices: the graph G whose edges are colored red, and its complement. This implies that Goodman's problem is to find the maximum value of $\sum_{i=1}^{n} d_i^2$ for $G \in \mathcal{G}(n,m)$. Olpp [63] gave some results on this problem. In 1999, Peled et al. [64] showed that the only possible graphs for which the maximum value is attained are the so-called *threshold graphs* and proved that all optimal graphs are in one of six classes of threshold graphs. Also in 1999, Byer [5] approached the problem in yet another equivalent context: he studied the maximum number of paths of length two over all graphs in $\mathcal{G}(n,m)$, which can be also transformed to the maximum value of $\sum_{i=1}^{n} d_i^2$. For this problem, there are also many results on the bounds and asymptotic values, see [17,19,47,57]. Finally, Àbrego et al. [1] completely solved this problem and determined all the graphs in $\mathcal{G}(n,m)$ attaining the maximum value of $\sum_{i=1}^{n} d_i^2$. Additionally, there are also some results on hypergraphs, as an example, see [6].

Another direction to studying the sum of the squares of degrees is the variance of degree sequence. For a graph G, let $Var(G)$ denote the variance of the degree sequence of G. Then

$$Var(G) = \frac{1}{n} \sum_{i=1}^{n} d_i^2 - d^2,$$

where $d = \frac{1}{n} \sum_{i=1}^{n} d_i$ is the average degree of G. In 1970, Erdös [31] firstly studied the variance of degrees of graphs. Actually, the variance of the degree sequence has some applications in social networks [65]. Independently, Snijders [65] studied the variance of the degree sequence too. For more results on this topic, we refer to [4,15,33,42].

For the general case, it seems that the first result on $\sum_{i=1}^{n} d_i^k$ was obtained by Székely et al. [73] in 1992. There are just a very few results on this topic, see [32,47]. In [33], the authors defined the k-th moment of the degree sequence of a graph G as $\mu_k(G) = \frac{1}{n} \sum_{n=1}^{n} d_i^k$, and then investigated the properties of μ_k.

Given a graph G whose degree sequence is $d_1, \ldots, d_n$, and for a real number $p > 0$, let

$$e_p(G) = \sum_{i=1}^{n} d_i^p.$$

Caro and Yuster [16] introduced a Turán-type problem for $e_p(G)$: for a given p, how large can $e_p(G)$ be if G has no subgraph of a particular type. Denote by $ex_p(n,H)$ the maximum value of $e_p(G)$ taken over all graphs with n vertices that do not contain H as a subgraph. Clearly, $ex_1(n,H) = 2ex(n,H)$. It is interesting to determine the value of $ex_p(n,H)$ and the corresponding extremal graphs. After this problem was proposed, many results comes out soon, see [9,10,37,62].

It is very likely that the sum of degree powers may find applications in computational chemistry and mathematical chemistry as a novel topological index. In general, a *topological index* is a single number that can be used to characterize structural properties of the graph representing a molecular network. Topological indices are numerical parameters of a graph which characterize its topology. Topological indices have been used for the development of quantitative structure–activity relationships (QSARs) in which the biological activity or other properties of molecules are correlated with chemical structures. More sophisticated topological indices also take the hybridization state of each of the atoms contained in the molecule into account. A short list of existing indices could be as follows. The Hosoya index [44] seems to be one of the first topological indices recognized in chemical graph theory. Other examples include the Wiener index [78,27], the Randić index [53,54,68], the Balaban index [3], the Gutman index [39], the Zagreb index [51], and graph energy [38,41,55]. For more results on topological indices, we refer to [40,49,50,75]. The just mentioned indices rely on invariants such as distances, vertex degrees, and eigenvalues. As mentioned, a challenging problem dealing with topological indices is to study the extremal (maximal and minimal) values of the indices for a given class of graphs. In view of the vast amount of existing graph measures, this area has been somewhat overlooked. Therefore, we would like to make an attempt in this direction by the present paper.

When discussing indices which are based on degree powers, the well-known Randić index [68] needs to be mentioned. In 1975, Randić [68] proposed a structural descriptor which is called *branching index* or *connectivity index*. For a (molecular) graph $G = (V,E)$, the Randić index $R(G)$ of G is defined as the sum of $(d(u)d(v))^{-1/2}$ over all edges uv of G, where $d(u)$ denotes the degree of a vertex u of G, i.e.,

$$R(G) = \sum_{uv \in E} (d(u)d(v))^{-1/2}.$$

The Randić index is the most used molecular descriptor in QSPR and QSAR, see [49,50]. The name connectivity index that replaced the term Randić index has been suggested by Kier, see [69]. Later in 1998 Bollobás and Erdös [8] generalized this index by replacing $-\frac{1}{2}$ with any real number α, which is called the *general Randić index*. Various mathematical results when investigating this quantity can be found in [53,54]. The Randić index has been extended as the general zeroth-order Randić index, and then the Zagreb indices appear to be the special cases of them. The zeroth-order Randić index, defined by Kier and Hall [51], is

$$^0R(G) = \sum_{u \in V(G)} d(u)^{-\frac{1}{2}}.$$

Later the zeroth-order general Randić index $^0R_\alpha(G)$ of a graph G has been defined as

$$^0R_\alpha(G) = \sum_{v \in V(G)} d(u)^\alpha$$

for any real number α. It should be noted that the same quantity is sometimes referred to as the "general first Zagreb index" [49,50], in view of the fact that $\sum_u (d(u))^2$ is sometimes called "the first Zagreb index". To study mathematical results for $^0R_\alpha(G)$, we refer to [45,46,53,54].

As an example and to get an idea of the complexity of the problem on finding the extremal values of degree-based measures, we state a result due to Li et al. [56] describing the extremal values of $\sum_{i=1}^n d_i^\alpha$ by using trees.

Proposition 1. *Among all trees of order n, for $\alpha > 1$ or $\alpha < 0$, the path and the star attain the minimum and maximum value of $\sum_{i=1}^n d_i^\alpha$, respectively; while for $0 < \alpha < 1$, the star graph and the path graph attain the minimum and maximum value of $\sum_{i=1}^n d_i^\alpha$, respectively.* □

4. Degree-based graph entropies

In order to start, we reproduce the definition of Shannon's entropy [70].

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

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

To define information-theoretic graph measures, we will often consider a tuple $(\lambda_1, \lambda_2, \ldots, \lambda_n)$ of non-negative integers $\lambda_i \in \mathbb{N}$ [20]. This tuple forms a probability distribution $p = (p_1, p_2, \ldots, p_n)$, where

$$p_i = \frac{\lambda_i}{\sum_{j=1}^{n} \lambda_j} \qquad i = 1, 2, \ldots, n.$$

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

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

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 [13], or partition-independent graph entropies, introduced by Dehmer [20,26], which are based on information functionals.

We are now ready to define the entropy of a graph due to Dehmer [20] by using information functionals.

Definition 2. Let $G = (V, E)$ be a connected graph. For a vertex $v_i \in V$, we define

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

where f represents an arbitrary information functional. □

Observe that $\sum_{i=1}^{|V|} p(v_i) = 1$. Hence, we can interpret the quantities $p(v_i)$ as vertex probabilities.

Now we immediately obtain one definition of a graph entropy of graph G.

Definition 3. Let $G = (V, E)$ be a connected graph and f be an arbitrary information functional. The entropy of G is defined as

$$I_f(G) = -\sum_{i=1}^{|V|} \frac{f(v_i)}{\sum_{j=1}^{|V|} f(v_j)} \log\left(\frac{f(v_i)}{\sum_{j=1}^{|V|} f(v_j)}\right) = \log\left(\sum_{i=1}^{|V|} f(v_i)\right) - \sum_{i=1}^{|V|} \frac{f(v_i)}{\sum_{j=1}^{|V|} f(v_j)} \log f(v_i). \quad \square \tag{2}$$

In the following, we define a novel information functional which is based on degree powers of graphs. We assume the order of the given graph to be n.

Definition 4. Let $G = (V, E)$ be a connected graph. For a vertex $v_i \in V$, we define the information functional as:

$$f := d_i^k,$$

where d_i is the degree of vertex v_i and k is an arbitrary real number. □

Therefore, by applying Definition 4 and Equality (2), we obtain the special graph entropy

$$I_f(G) = -\sum_{i=1}^{n} \frac{d_i^k}{\sum_{j=1}^{n} d_j^k} \log\left(\frac{d_i^k}{\sum_{j=1}^{n} d_j^k}\right) = \log\left(\sum_{i=1}^{n} d_i^k\right) - \sum_{i=1}^{n} \frac{d_i^k}{\sum_{j=1}^{n} d_j^k} \log d_i^k. \tag{3}$$

In this paper, we will discuss the extremal properties of the above graph entropy based on degree powers. We discuss some applications in Section 7.

5. Extremal properties of certain graphs for $k = 1$

In this section, we suppose $k = 1$ and we will obtain results regarding the maximum and minimum entropy by using certain families of graphs. Let $G = (V, E)$ be a graph with n vertices and m edges. Observe that

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

From Equality (3), we infer

$$I_f(G) = \log\left(\sum_{i=1}^{n} d_i\right) - \sum_{i=1}^{n} \frac{d_i}{\sum_{j=1}^{n} d_j} \log d_i = \log(2m) - \frac{1}{2m}\sum_{i=1}^{n} (d_i \log d_i). \tag{4}$$

Therefore, for a class of graphs with given number of edges, the extremal values of $I_f(G)$ are only determined by the extremal values of $\sum_{i=1}^{n} (d_i \log d_i)$.

Now we define a function $h(G) = \sum_{i=1}^{n} (d_i \log d_i)$. In the following, we will study the extremal values of $h(G)$ for certain classes of graphs, from which we can easily obtain the extremal values of the graph entropy.

To start we state some notation. Denote by $D(G) = [d_1, d_2, \ldots, d_n]$ the degree sequence of G, and $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$. If there is a graph G with $D(G) = [d_1, d_2, \ldots, d_n]$ such that $d_i \geqslant d_j + 2$, then let G' be the graph obtained from G by replacing the pair (d_i, d_j) by the pair $(d_i - 1, d_j + 1)$, that is, $D(G') = [d_1, d_2, \dots, d_{i-1}, d_i - 1, d_{i+1}, \dots, d_{j-1}, d_j + 1, d_{j+1}, \dots, d_n]$. Finally we state a lemma.

Lemma 1. *For graphs G and G', specified above, we have $h(G) > h(G')$.*

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

$$\begin{aligned} h(G) - h(G') &= d_i \log d_i + d_j \log d_j - (d_i - 1)\log(d_i - 1) - (d_j + 1)\log(d_j + 1) \\ &= (d_i \log d_i - (d_i - 1)\log(d_i - 1)) - ((d_j + 1)\log(d_j + 1) - d_j \log d_j) \\ &= \left(\log \xi_1 + \frac{1}{\ln 2}\right) - \left(\log \xi_2 + \frac{1}{\ln 2}\right) > 0, \end{aligned}$$

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

Thus, the proof is completed. $\square$

5.1. Trees

Lemma 2. *Let T be a tree of order n. Then $h(T) \geqslant h(P_n)$, the equality holds if and only if $T \cong P_n$; and $h(T) \leqslant h(S_n)$, the equality holds if and only if $T \cong S_n$.*

Proof. Let T be a tree of order n and let its degree sequence be $d_1, d_2, \dots, d_n$. It is not difficult to see that if $T \ncong P_n$, then there must exist a pair (d_i, d_j) such that $d_i \geqslant d_j + 2$. We construct a tree T' by replacing the pair (d_i, d_j) by the pair $(d_i - 1, d_j + 1)$. Then by Lemma 1, we obtain that $h(T) > h(T')$. Repeating the above operation until there is no pair (d_i, d_j) such that $d_i \geqslant d_j + 2$ for all i, j, we obtain a tree sequence $T, T', T'_1, \dots, T'_s$ such that $T'_s \cong P_n$. Clearly, $h(T) > h(T') > \cdots > h(T'_s)$. Thus, for any tree $T \ncong P_n$, $h(T) > h(P_n)$.

Using Lemma 1 and by a similar discussion, we can show that if T is a tree of order n, then $h(T) \leqslant h(S_n)$, the equality holds if and only if $T \cong S_n$. $\square$

From the above lemma and Equality (4), we get the following result towards extremal properties of the graph entropy.

Theorem 1. *Let T be a tree with n vertices and $k = 1$. Then we have $I_f(T) \leqslant I_f(P_n)$, the equality holds if and only if $T \cong P_n; I_f(T) \geqslant I_f(S_n)$, the equality holds if and only if $T \cong S_n$.* $\square$

5.2. Unicyclic graphs

Lemma 3. *Let G be a unicyclic graph of order n. Then we have $h(G) \geqslant h(C_n)$, the equality holds if and only if $G \cong C_n; h(G) \leqslant h(S_n^+)$, the equality holds if and only if $G \cong S_n^+$.*

Proof. We do the proof by contradiction. Suppose G attains the minimum value among all unicyclic graphs and $G \ncong C_n$. Let $C = v_1 v_2 \dots v_t v_1$ be the unique cycle in G. Then $t < n$ and there is at least one vertex v_i with degree $d_i \geqslant 3$. Without loss of generality, we assume $d_1 \geqslant 3$. Let $P = v_1 u_1 u_2 \dots u_s$ be a longest path in $G \setminus C$ starting at v_1, i.e., $u_i \notin C$. Obviously, $d(u_s) = 1$. Let $G' = G - v_1 v_2 + v_2 u_s$. Then by Lemma 1, we obtain $h(G) > h(G')$, which contradicts to the choice of G. $\square$

Now suppose G attains the maximum value among all unicyclic graphs. Let $C = v_1 v_2 \dots v_t v_1$ be the unique cycle in G.

Claim 1. There is at least one vertex $v_i \in C$ with the maximum degree $\Delta(G)$.

Proof. Suppose there is no vertex on the cycle C possessing the maximum degree. Choose a vertex v satisfying that $d(v) = \Delta(G)$. Let $P = v_i u_1 u_2 \dots u_s$ be a longest path in $G \setminus C$ starting at v_i such that the vertex v is on the path. We construct a new graph $G' = G - v_i v_{i+1} + v_{i+1} v$. Then by Lemma 1, we infer $h(G') > h(G)$, a contradiction. $\square$

Claim 2. $|V(C)| = 3$.

Proof. Now suppose $d(v_1) = \Delta(G)$. If $|V(C)| = 4$, then let $G' = G - v_3 v_4 + v_1 v_3$. Then by Lemma 1, we obtain $h(G') > h(G)$, which contradicts to the choice of G. $\square$

Claim 3. $\Delta(G) = n - 1$.

Proof. Suppose $d(v_1) = \Delta(G)$. Obviously, $\Delta(G) > 2$. If $\Delta(G) \leqslant n - 2$, then by Claims 1 and 2, there is at least one vertex $v \in V(G)$ with $d(v) = 1$ and $v_1 v \notin E(G)$. Let w be the unique neighbor of v and let $G' = G - vw + v_1 v$. Then by Lemma 1, we obtain $h(G') > h(G)$, a contradiction.

From the above three claims, we can easily obtain that $h(G)$ attains the maximum value if and only if $G \cong S_n^+$. $\square$

From the above lemma and Equality (4), we can obtain the following result on the extremal properties of the graph entropy.

Theorem 2. *Let G be a unicyclic graph with n vertices and $k = 1$. Then we have $I_f(G) \leqslant I_f(C_n)$, the equality holds if and only if $G \cong C_n$; $I_f(G) \geqslant I_f(S_n^+)$, the equality holds if and only if $G \cong S_n^+$.* □

5.3. Bicyclic graphs

Let G^* be a bicyclic graph with degree sequence $[3^2, 2^{n-2}]$. Denote by G^{**} the bicyclic graph with degree sequence $[n-1, 3, 2^2, 1^{n-4}]$.

Lemma 4. *Let G be a bicyclic graph of order n. Then we have $h(G) \geqslant h(G^*)$, the equality holds if and only if $G \cong G^*$; and $h(G) \leqslant h(G^{**})$, the equality holds if and only if $G \cong G^{**}$.*

Proof. We do the proof by contradiction. Suppose G attains the minimum value among all bicyclic graphs. We claim that the minimum degree fulfills $\delta(G) \geqslant 2$. Otherwise, let v_0 be a vertex with degree 1 and assume $P = v_0v_1v_2 \ldots v_s$ is a path with $d(v_s) \geqslant 3$ and $d(v_i) = 2$ for $i = 1, 2, \ldots, s-1$. Let G' be the graph obtained from G by deleting vertices $v_0, v_1, \ldots, v_{s-1}$ and inserting s new vertices into an edge of a cycle of G. Then by Lemma 1, we obtain $h(G) > h(G\prime)$, a contradiction. Again by using Lemma 1, we easily obtain that among all bicyclic graphs, $h(G)$ attains the minimum value if and only if $G \cong G^*$.

Now suppose G attains its maximum value among all bicyclic graphs. Let u be a vertex of the maximum degree. We claim that if G contains some vertex v with degree 1, then $uv \in E(G)$. Otherwise, we construct a new graph $G' = G + uv - vw$, where w is the unique neighbor of v. Then by Lemma 1, we can obtain that $h(G') > h(G)$, a contradiction. Next, we will show that u is a common vertex of all the cycles of G. Otherwise, assume u does not lie on the cycle C of G. Let P be a path connecting u to C such that $V(C) \cap V(P) = \{v\}$. Let w be a vertex of C with $vw \in E(C)$. Set $G' = G + uw - vw$. Then by Lemma 1, we infer $h(G') > h(G)$, a contradiction. Based on the above two properties, we discuss three cases of bicyclic graphs: graphs having two cycles without common vertices, graphs having two cycles with only one common vertex, and those having two cycles with more than one common vertices. Again by using Lemma 1, we easily obtain that among all bicyclic graphs, $h(G)$ attains the maximum value if and only if $G \cong G^{**}$. □

From the above lemma and Equality (4), we finally get the following result towards the extremal properties of the graph entropy.

Theorem 3. *Let G be a bicyclic graph with n vertices and $k = 1$. Then we have $I_f(G) \leqslant I_f(G^*)$, the equality holds if and only if $G \cong G^*$; $I_f(G) \geqslant I_f(G^{**})$, the equality holds if and only if $G \cong G^{**}$.* □

5.4. Chemical trees

In this subsection, we consider chemical trees. By performing a numerical analysis, we observed that a special tree attains the maximum value of h. We define this tree T^* as follows: T^* is a tree with n vertices and $n-2 = 3a+i$, $i = 0, 1, 2$, whose degree sequence is $D(T^*) = [4^a, i+1, 1^{n-a-1}]$.

Lemma 5. *Let T be a chemical tree of order n and $n-2 = 3a+i$, $i = 0, 1, 2$. Then we get $h(T) \leqslant h(T^*)$, the equality holds if and only if $T \cong T^*$.*

Proof. Let T be a chemical tree of order n with degree sequence $D(T) = [d_1, d_2, \ldots, d_n]$. If there exists a pair (d_i, d_j) such that $4 > d_i \geqslant d_j \geqslant 2$, then we can construct a new tree T_1 by replacing the pair (d_i, d_j) by (d_i+1, d_j-1). By Lemma 1, we obtain $h(T_1) > h(T)$. Repeating the above operations until there is no such pair, we obtain a new tree T', which has some vertices of degree 4, some vertices of degree 1, and at most one vertex of degree 2 or degree 3. Now we denote by a, b, c, d the number of the vertices of degrees $4, 3, 2, 1$, respectively. Then we have

$$\begin{cases} 4a + 3b + 2c + d = 2n - 2 \\ a + b + c + d = n \\ b + c \leqslant 1. \end{cases}$$

From the above expressions, we infer the following solutions:

(1) If $n-2 \equiv 0 (mod\ 3)$, then $a = \frac{n-2}{3}, b = c = 0, d = n-a$.
(2) If $n-2 \equiv 1 (mod\ 3)$, then $a = \frac{n-3}{3}, b = 0, c = 1, d = n-a-1$.
(1) If $n-2 \equiv 2 (mod\ 3)$, then $a = \frac{n-4}{3}, b = 1, c = 0, d = n-a-1$.

Thus, the proof is completed. □

Observe that the path graph is also a chemical tree. Then from Theorem 1, we know that P_n attains the maximum value of I_f among all chemical trees. Therefore, from the above lemma and Equality (4), we can obtain the following result on the extremal properties of the graph entropy.

Theorem 4. *Let T be a chemical tree with n vertices such that $n-2=3a+i$, $i=0,1,2$, and $k=1$. Then we have $I_f(T) \leqslant I_f(P_n)$, the equality holds if and only if $T \cong P_n$; $I_f(T) \geqslant I_f(T^*)$, the equality holds if and only if $T \cong T^*$.* □

5.5. Chemical graphs

In this subsection, we will consider the extremal values of general chemical graphs with n vertices and m edges, which is called (n,m)-*chemical graphs*. Before we state our results, we will define two special graphs. Let G_1 be the (n,m)-chemical graph with degree sequence $[d_1,d_2,\ldots,d_n]$, such that $|d_i-d_j| \leqslant 1$ for any $i \neq j$. Let G_2 be a (n,m)-chemical graph with at most one vertex of degree 2 or 3.

Lemma 6. *Let G be an (n,m)-chemical graph. Then we have $h(G) \geqslant h(G_1)$, the equality holds if and only if $G \cong G_1$.*

Proof. Let G be a chemical graph and $D(G)=[d_1,d_2,\ldots,d_n]$ such that $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$. If $G \ncong G_1$, then there must be a pair (d_i,d_j) such that $d_i \geqslant d_j+2$. By Lemma 1, there is a graph G' by replacing the pair (d_i,d_j) by the pair (d_i-1,d_j+1), which has a larger value than that of G_1. □

To show the existence, we get the extremal (n,m)-graph G_1 by adding edges one by one. Firstly, we start from a tree. There must be at least two leaves in a tree. By Lemma 1, there does not exist any 3-degree vertex, so the extremal tree must be a path P_n, which can also be obtained from Lemma 2. Then we add an edge connecting the two leaves of path P_n. In this way, the degree of the vertices are all equal to two, and then we get a cycle. Then we add edges one by one, so as to maximize the number of 3-degree vertices, until there is no 2-degree vertices. At last, we add edges arbitrarily as long as no vertex gets degree more than 4.

Lemma 7. *Let G be an (n,m)-chemical graph. Then we have $h(G) \leqslant h(G_2)$ for $m=n-1$ and $m \geqslant n \geqslant 8$, the equality holds if and only if $G \cong G_2$.*

Proof. Let G be an (n,m)-chemical graph and $D(G)=[d_1,d_2,\ldots,d_n]$. If $G \ncong G_2$, then there must have at least two vertices of degree 2 or 3, i.e., there is a pair (d_i,d_j) such that $3 \geqslant d_i \geqslant d_j \geqslant 2$. By Lemma 1, there is a graph G' by replacing the pair (d_i,d_j) by the pair (d_i+1,d_j-1), and G' has a maximum value than that of G. Repeating the above operations until there is no pair (d_i,d_j) such that $3 \geqslant d_i \geqslant d_j \geqslant 2$, we can get the graph G_2 with the maximum value. □

In the following, we will show the existence of graph G_2. Denote by n_i the number of vertices of degree i in a chemical graph, $i=1,2,3,4$. For graph G_2, we have

$$\begin{cases} n_1+n_2+n_3+n_4=n \\ n_1+2n_2+3n_3+4n_4=2m \\ n_2+n_3 \leqslant 1 \end{cases}$$

From the above equations, we infer

(1) $n_2=n_3=0$, and $n_1=\frac{4n-2m}{3}$, $n_4=\frac{2m-n}{3}$, if $2m-n \equiv 0 \pmod 3$;
(2) $n_2=1, n_3=0$, and $n_1=\frac{4n-2m-2}{3}$, $n_4=\frac{2m-n-1}{3}$, if $2m-n \equiv 1 \pmod 3$;
(3) $n_2=0, n_3=1$, and $n_1=\frac{4n-2m-1}{3}$, $n_4=\frac{2m-n-2}{3}$, if $2m-n \equiv 2 \pmod 3$.

To show the existence, we can construct G_2 by this way.
Case 1. $n=m-1$.

(i) If $2m-n \equiv 0 \pmod 3$, we construct a path with n_4 vertices first, and then add n_1 pendent vertices, as long as no vertex gets degree more than 4;
(ii) If $2m-n \equiv 1 \pmod 3$, we construct a path with n_4 vertices first, and then add n_1 pendent vertices, as long as no vertex gets degree more than 4, finally subdivide an edge;
(iii) If $2m-n \equiv 2 \pmod 3$, we construct a path with n_4+1 vertices first, and then add n_1 pendent vertices, as long as no vertex gets degree more than 4.

Case 2. $m \geqslant n \geqslant 8$.
For $n_4 \geqslant 5$, that is $\lfloor \frac{2m-n}{3} \rfloor \geqslant 5$, we can construct G_2 in the following way.

(i) If $2m-n \equiv 0 \pmod 3$, we construct a 4-regular graph on n_4 vertices first, and then delete $\frac{n_1}{2}$ edges and add n_1 pendent vertices, as long as no vertex gets degree more than 4;
(ii) If $2m-n \equiv 1 \pmod 3$, we construct a 4-regular graph on n_4 vertices first, and then delete $\frac{n_1}{2}$ edges and add n_1 pendent vertices, as long as no vertex gets degree more than 4, finally subdivide an edge;

(iii) If $2m - n \equiv 2 \ (mod\ 3)$, we construct a 4-regular graph on $n_4 + 1$ vertices first, and then delete $\frac{n_1+1}{2}$ edges and add n_1 pendent vertices, as long as no vertex gets degree more than 4.

For $n_4 \leqslant 4$, there are only some pairs of (n, m), which can be listed easily.

Therefore, from the above two lemmas and Equality (4), we can obtain the following result on the extremal properties of the graph entropy.

Theorem 5. *Let G be an (n, m)-chemical graph and $k = 1$. Then we have $I_f(G) \leqslant I_f(G_1)$, the equality holds if and only if $G \cong G_1; I_f(G) \geqslant I_f(G_2)$, the equality holds if and only if $G \cong G_2$.* □

6. Extremal properties for $k > 0$

It seems challenging to consider the general case $k > 0$ by directly using the method in Section 5, since the exact value of $\sum_{i=1}^{n} d_i^k$ changes when we replace the pair (d_i, d_j) by $(d_i - 1, d_j + 1)$.

By performing numerical experiments, we obtained the following conjecture. Unfortunately, several attempts to prove the statement by using different methods failed.

Conjecture 1. *Let T be a tree with n vertices and $k > 0$. Then we have $I_f(T) \leqslant I_f(P_n)$, the equality holds if and only if $T \cong P_n; I_f(T) \geqslant I_f(S_n)$, the equality holds if and only if $T \cong S_n$.* □

In the following, we give some ideas how to prove the result. Firstly, we present one general property on entropy measures, which seems simple but very useful. This result is applicable for any Shannon's entropy, but not necessarily graph entropy measures. In particular, we study the behavior of the entropy function when the probability vector p or the underlying tuple $(\lambda_1, \lambda_2, \ldots, \lambda_n)$ is altered.

Take $\sum_{i=1}^{n} \lambda_i$ as an single variant and let $y = \sum_{i=1}^{n} \lambda_i$. Then Equality (1) can be transformed into

$$I = \log y - \frac{1}{y} \sum_{i=1}^{n} \lambda_i \log \lambda_i = \log y - \frac{g(y)}{y},$$

where $g(y) = \sum_{i=1}^{n} \lambda_i \log \lambda_i$.

Proposition 2. *Suppose $I = \log y - \frac{g(y)}{y}$.*

(i) *If I is a monotonously increasing function on y, then the maximum (minimum) value of I can be achieved when y attains its maximum (minimum) value.*
(ii) *If I is a monotonously decreasing function on y, then the maximum (minimum) value of I can be achieved when y attains its minimum (maximum) value.* □

For the graph entropy defined by Equality (3), we can let $y = \sum_{i=1}^{n} d_i^k$. Then we have

$$I = \log y - \frac{1}{y} \sum_{i=1}^{n} d_i^k \log d_i^k = \log y - \frac{g(y)}{y},$$

where $g(y) = \sum_{i=1}^{n} d_i^k \log d_i^k$. However, we have not been able to find the efficient relation between $g(y)$ and y.

Some numerical results support that if $k > 0$, then I is a monotonously decreasing function on y for trees, from which together with Proposition 1 we easily obtain the results of Conjecture 1.

Conjecture 2. *For $k > 1$, I is a monotonously decreasing function on y for trees; while for $0 < k < 1$, I is a monotonously increasing function on y for trees.* □

7. Application of degree-based entropies

Entropy measures for graphs have been widely applied in biology, computer science and structural chemistry, see, e.g., [11,24–26]. Broadly speaking, the applications for entropic network measures range from quantitative structure characterization in structural chemistry or software technology to explore biological or chemical properties of molecular graphs. We emphasize that the just mentioned applications relate to solve an underlying data analysis problem, e.g., a clustering or classification task. However, the so-called structural interpretation needs to be investigated as well. This calls to examine what kind of structural complexity does the measure detect. This problem is intricate as it is not clear on which graph class the measure should be evaluated. We conjecture that the introduced degree-based entropy can be used to measure network heterogeneity. Similar entropic measures which are based on vertex-degrees to detect network heterogeneity have been introduced by Solé [66] and Tan and Wu [74].

8. Summary and conclusion

Several graph invariants have been used for constructing entropy-based measures to determine the complexity of networks. Based on Shannon's entropy, we have studied the graph entropy, which is based on an information functional by using degree powers. As reported by Dehmer and Kraus [23], there is a lack of analytical results when proving extremal results for entropy-based graph measures. In this paper, we proved extremal results for the just mentioned graph entropy. For $k = 1$, we characterized the graphs which attains the maximum or minimum values among certain classes of graphs, namely, trees, unicyclic graphs, bicyclic graphs, chemical trees and chemical graphs. For the general case $k > 0$, we express some conjectures generated by numerical simulations to find extremal values of trees.

Actually, we do not discuss the case of $k < 0$, since this case is very complicated. By some elementary calculations, we find that the extremal graphs will not be unique. As an example, we will consider the extremal results on trees with at most nine vertices for different values of k. In the following, for convenience, we use "*minimum (maximum) graph*" instead of "the graphs attaining the minimum (maximum) value of graph entropy".

For $k = -1/2$, the minimum graphs and the maximum graphs for $5 \leqslant n \leqslant 9$ are listed in the following table, respectively.

n	Maximum graph	Minimum graph (Number of minimum graphs)
5	P_n	S_n
6	P_n	S_n
7	P_n	Trees with degree sequence $[4, 3, 1^5]$ (1 graph)
8	P_n	Trees with degree sequence $[4^2, 1^6]$ (1 graph)
9	P_n	Trees with degree sequence $[5, 4, 1^7]$ (1 graph)

For $k = -1$, the minimum graphs and the maximum graphs for $5 \leqslant n \leqslant 9$ are listed in the following table, respectively.

n	Maximum graph	Minimum graph (Number of minimum graphs)
5	P_n	S_n
6	P_n	Trees with degree sequence $[3^2, 1^4]$ (1 graph)
7	P_n	Trees with degree sequence $[4, 3, 1^5]$ (1 graph)
8	P_n	Trees with degree sequence $[3^3, 1^5]$ (1 graph)
9	P_n	Trees with degree sequence $[4, 3^2, 1^6]$ (2 graphs)

For $k = -2$, the minimum graphs and the maximum graphs for $5 \leqslant n \leqslant 9$ are listed in the following table, respectively.

n	Maximum graph	Minimum graph (Number of minimum graphs)
5	S_n	Trees with degree sequence $[3, 2, 1^3]$ (1 graph)
6	S_n	Trees with degree sequence $[3, 2^2, 1^3]$ (2 graphs)
7	S_n	Trees with degree sequence $[3, 2^3, 1^3]$ (3 graphs)
8	S_n	Trees with degree sequence $[3^2, 2^2, 1^4]$ (5 graphs)
9	S_n	Trees with degree sequence $[3^2, 2^3, 1^4]$ (9 graphs)

In the future, we will continue to study extremal values of graph entropies for some special classes of graphs as well as for more general graphs. We are going to tackle this problem for $k < 0$ too. The structural interpretation of these measures will be also explored. In the mathematical literature, tackling this problem has been overlooked. Also, we intend to employ the measure $I_f(G)$ to determine the similarity/distance of graphs by employing known similarity/distance measures. To do so, one needs to first study mathematical properties of the graph measures as we did in this paper. Hence, the paper can be also seen as a preliminary study for working on the latter problem.

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