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Graph Operations Decreasing Values of Degree-Based Graph Entropies

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Abstract

The degree-based graph entropy I_d is a parametric measure derived from an information functional defined by vertex degrees of a graph, which is used to characterize the structure of complex networks. Determining minimal values of I_d is challenging due to a lack of effective methods to analyze properties of minimal graphs. In this paper, we investigate minimal properties of the graph entropy in (n, m)-graphs and define two new graph operations, which can decrease the values of I_d.

1 Introduction

Graph entropies are useful measures of the complexity of a system described as a graph. There have been various graph entropies in different applications [5] to play different roles. Among them, Dehmer [4] presented a framework for constructing new entropies based on information functionals, aiming to infer and characterize the relational structure of complex

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networks. Therefore, many graph invariants were employed to define information functionals [1, 8, 9]. And as a consequence, degree-based graph entropies [2] have been introduced and have begun to draw the attention of researchers in information theory, graph theory, and mathematical chemistry.

Let G be an (n, m)-graph, that is, with n vertices and m edges, and the vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. Let $d_G(v_i)$ or $d(v_i)$ denote the degree of v_i. We refer the reader to [2] for further details about the degree-based graph entropy and only present the simplified definition.

Definition 1. The degree-based entropy of G is defined as

$$I_d(G) = \log(2m) - \frac{1}{2m} \sum_{i=1}^{n} d(v_i) \log d(v_i).$$

The logarithms are always taken to the base two in this paper. And for the purposes of this discussion, let $f(d(v_i)) = d(v_i) \log d(v_i)$ and $h(G) = \sum_{i=1}^{n} f(d_i)$. Then $I_d(G) = \log(2m) - \frac{1}{2m} h(G)$ and the minimum value of $I_d(G)$ can be easily obtained from the maximum value of $h(G)$.

In [2], the authors studied extremal properties of I_d and obtained the extremal values of trees, unicyclic graphs, and bicyclic graphs. Das and Shi [3] gave an upper bound of graph entropies based on degree powers, a generalization of I_d, for graphs with given numbers of vertices and a lower bound for trees. It is more challenging to determine minimal values of graph entropies due to a lack of effective methods to tackle this problem [6]. The maximum values of I_d were obtained for (n, m)-bipartite graphs in [7]. Then Yan determined the graphs attaining the maximum values in all (n, m)-graphs, and the structure of the graphs attaining the minimum values was described as a certain family of graphs, namely K_aT graphs.

Based on the work in [10], we conduct further research into the properties of K_aT graphs and define two new graph operations, which decrease the values of I_d. It means that the operations can be effective tools to study extremal properties of graph entropies for general graphs.

2 Graph operations

The *neighbor set* $N_G(v)$ or $N(v)$ of a vertex v in G is the set of all vertices adjacent to v. Clearly, the degree of v in G is the size of $N(v)$. A *complete graph* K_n is a graph with n vertices such that all the vertices are pairwise adjacent. A graph with no edges is called an *empty graph*.

In [10], a certain family of graphs named K_aT graphs were introduced, and the graphs attaining the maximum values of h were proved isomorphic to such graphs. Recall that $I_d(G) = \log(2m) - \frac{1}{2m}h(G)$. Next, we reproduce the results as a start.

Definition 2. A K_aT *graph* is one whose vertex set can be partitioned into two disjoint sets S and T, where $|S| = a$, so that S and T induce a complete graph K_a and an empty graph, respectively, if $d(t_i) \geq d(t_j)$ for $t_i, t_j \in T$, then $N(t_j) \subseteq N(t_i)$.

Theorem 1. *Any connected graph attaining the maximum value of h must be isomorphic to a K_aT graph.*

Obviously, a K_aT graph with $a = 1$ or 2 is a tree. Since only connected (n, m)-graphs that are not trees are considered, we assume $a \geq 3$ in this paper. In addition, if there is a vertex with degree a in T, we still get a graph with such structure after removing the vertex from T and adding it to K_a. So it is feasible to assume that $d(t) \leq a - 1$ for any $t \in T$ in a K_aT graph. For simplicity and clarity of exposition, we will refer to T as the independent set instead of a specified set in any K_aT graph. $V(K_a)$ denotes the set of vertices in K_a.

As an immediate result, the following lemma will be of considerable use.

Lemma 1. *Let G be a K_aT graph, $V(K_a) = \{v_1, v_2, \ldots, v_a\}$, and suppose that $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_a)$. Then*
(1) $N(t) = \{v_1, v_2, \ldots, v_{d(t)}\}$ for any vertex $t \in T$;
(2) v_i is adjacent to all the vertices whose degrees are not less than i in T.

Proof. To prove (1), suppose, on the contrary, that there exists a vertex $t \in T$ such that $v_i \in N(t)$ and $v_j \notin N(t)$, where $d(t) + 1 \leq i \leq a - 1$ and

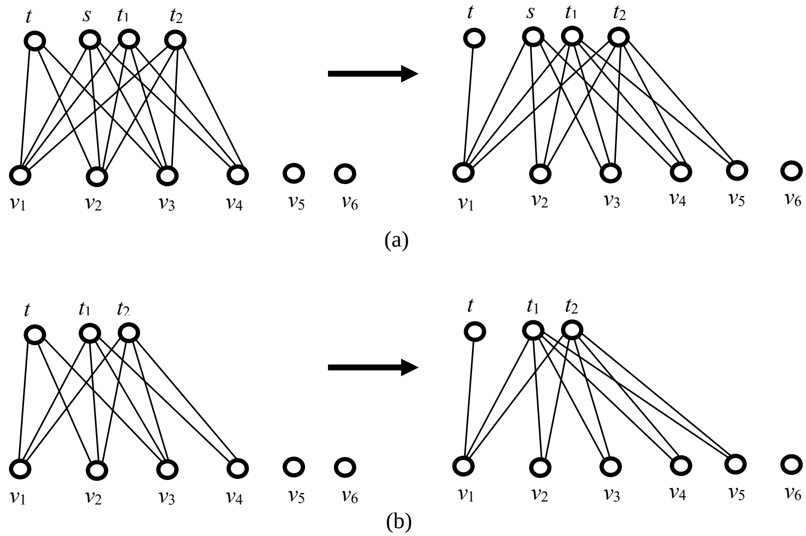

Figure 1. 2-edge distributions from t to t_1, t_2

$1 \leq j \leq d(t)$. Then we have $d(v_i) \leq d(v_j)$ for $i > j$, which means that there must exist another vertex s in T such that v_j is adjacent to s, but v_i is not. Therefore $N(t) \not\subseteq N(s)$ and $N(s) \not\subseteq N(t)$, which contradicts the definition of K_aT graphs. Clearly, (2) is immediate by (1). ■

Next, we define two graph operations in K_aT graphs, which are asserted by Lemmas 2 and 3.

Definition 3. Let G be a K_aT graph, $V(K_a) = \{v_1, v_2, \ldots, v_a\}$, and suppose $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_a)$. If there are vertices $t, t_1, t_2, \ldots, t_k$ in T such that $k + 1 \leq d = d(t) \leq d(t_1) = d(t_2) = \cdots = d(t_k) = d'$, then the operations of deleting the edges $tv_d, tv_{d-1}, \ldots, tv_{d-k}$ and adding the edges $t_1v_{d'+1}, t_2v_{d'+1}, \ldots, t_kv_{d'+1}$ in G are called a k-edge distribution from t to $t_1, t_2, \ldots, t_k$. The distribution is proper if there is no vertex of T with degree greater than $d - k$ and less than $d' + 1$ in the resulting graph.

The definition seems a little intricate, but by combining Lemma 1, we can present the procedure of the k-edge distribution from t to $t_1, t_2, \ldots, t_k$ in an intuitive way. First, arrange the vertices of K_a in a row in descending order of their degrees; then take away k edges incident with t from back

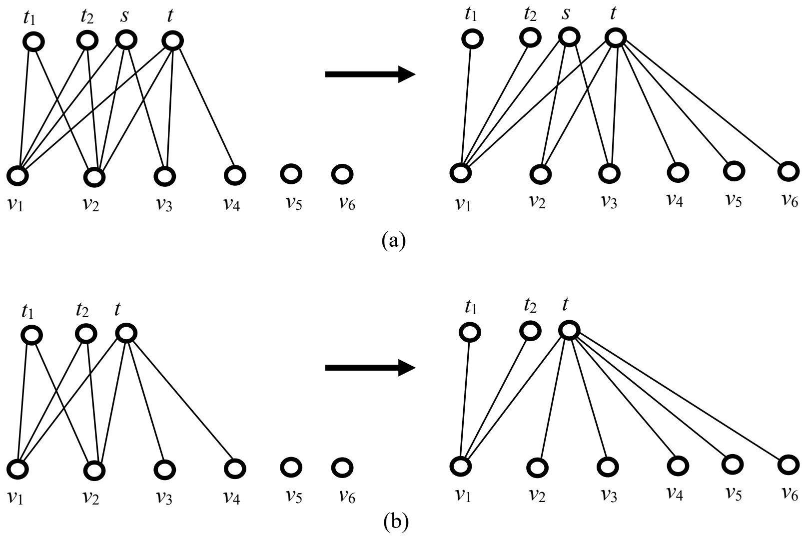

Figure 2. 2-edge accumulations from t_1, t_2 to t

to front; add an edge between each t_i and the first vertex nonadjacent to t_i, $i = 1, 2, \ldots, k$. Figure 1 illustrates distributions from t to t_1, t_2 in two K_aT graphs, where (b) is proper and (a) is not. Note that the edges in K_a are omitted from the figure for brevity.

Definition 4. Let G be a K_aT graph, $V(K_a) = \{v_1, v_2, \ldots, v_a\}$, and suppose $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_a)$. If there are vertices $t_1, t_2, \ldots, t_k, t$ in T such that $2 \leq d' = d(t_1) = d(t_2) = \cdots = d(t_k) \leq d(t) = d \leq a - k$, then the operations of deleting the edges $t_1v_{d'}, t_2v_{d'}, \ldots, t_kv_{d'}$ and adding the edges $tv_{d+1}, tv_{d+2}, \ldots, tv_{d+k}$ in G are called a k-edge accumulation from $t_1, t_2, \ldots, t_k$ to t. The accumulation is proper if there is no vertex of T with degree greater than $d' - 1$ and less than $d + k$ in the resulting graph.

The two examples of 2-edge accumulations given in Figure 2 are both from t_1, t_2 to t, but (b) is proper and (a) is not. It will be convenient to refer to a 'k-edge distribution' as a *distribution* and a 'k-edge accumulation' as an *accumulation*. It is easy to see that in either operation, edges are moved from vertices with smaller degrees to vertices with larger degrees. $G - uv$ and $G + uv$ denote the graphs obtained by deleting and adding the edge uv in G.

Lemma 2. *The graph obtained by performing a distribution in a K_aT graph is also a K_aT graph.*

Proof. Let G be a K_aT graph and $V(K_a) = \{v_1, v_2, \cdots, v_a\}$ with $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_a)$. Let G' be the graph obtained by a distribution from t to $t_1, t_2, \ldots, t_k$ in G, where $k+1 \leq d = d(t) \leq d(t_1) = d(t_2) = \cdots = d(t_k) = d'$. By definition, we have

$$G' = G - tv_d - tv_{d-1} - \cdots - tv_{d-k+1} + t_1v_{d'+1} + t_2v_{d'+1} + \cdots + t_kv_{d'+1}.$$

Since $N_G(t) = \{v_1, v_2, \ldots, v_d\}$ and $N_G(t_i) = \{v_1, v_2, \ldots, v_{d'}\}$ by part (1) of Lemma 1, $N_{G'}(t) = \{v_1, v_2, \ldots, v_{d-k}\}$ and $N_{G'}(t_i) = \{v_1, v_2, \ldots, v_{d'+1}\}$, $i = 1, 2, \ldots, k$. Then for any $s \in T$, $N_{G'}(s) = \{v_1, v_2, \ldots, v_{d_{G'}(s)}\}$. Clearly, $N_{G'}(u) \subseteq N_{G'}(v)$ for any vertices u and v with $d_{G'}(u) \leq d_{G'}(v)$, and hence G' is a K_aT graph. ■

Lemma 3. *The graph obtained by performing an accumulation in a K_aT graph is also a K_aT graph.*

Proof. The proof of this lemma is analogous to that of Lemma 2. ■

3 Minimal properties of I_d

The following two theorems show that both a proper distribution and a proper accumulation are operations that increase the values of h.

Theorem 2. *Let G' be a graph obtained by performing a proper distribution in K_aT graph G. Then $h(G') > h(G)$.*

Proof. Let $t, t_1, t_2, \ldots, t_k$ be vertices in T of G, $k \geq 1$, such that

$$k+1 \leq d = d(t) \leq d(t_1) = d(t_2) = \cdots = d(t_k) = d'.$$

Let $V(K_a) = \{v_1, v_2, \ldots, v_a\}$ with $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_a)$. Assume that the distribution from t to $t_1, t_2, \ldots, t_k$ is proper, and G' is the resulting graph. By Lemma 2, G' is a K_aT graph. Then we have

$$G' = G - tv_d - tv_{d-1} - \cdots - tv_{d-k+1} + t_1v_{d'+1} + t_2v_{d'+1} + \cdots + t_kv_{d'+1}.$$

Recall that $f(d(v_i)) = d(v_i)\log d(v_i)$ and $h(G) = \sum_{i=1}^{n} f(d_i)$. Let

$$A = f(d) - f(d-k); \qquad B = f(d(v_{d'+1}) + k) - f(d(v_{d'+1}));$$
$$C = k[f(d'+1) - f(d')]; \qquad D = \sum_{i=d-k+1}^{d} [f(d(v_i)) - f(d(v_i) - 1)].$$

Then,

$$h(G) - h(G') = (A - C) - (B - D). \tag{1}$$

Now we claim that $d(v_{d-k+1}) = d(v_{d'+1}) + k + 1$ in G. Since the distribution is proper, there is no vertex of T with degree greater than $d-k$ and less than $d'+1$ in G'. Therefore, by part (2) of Lemma 1, $d_{G'}(v_{d-k+1}) = d_{G'}(v_{d'+1})$, and so $d(v_{d-k+1}) = d(v_{d'+1}) + k + 1$. Then we have the inequality:

$$d(v_d) \leq d(v_{d-1}) \leq \cdots \leq d(v_{d-k+1}) = d(v_{d'+1}) + k + 1.$$

Because $f(x) - f(x-1)$ is an increasing function,

$$D \leq k[f(d(v_{d'+1}) + k + 1) - f(d(v_{d'+1}) + k)]. \tag{2}$$

In addition, since $d \leq d'$,

$$C \geq k[f(d+1) - f(d)]. \tag{3}$$

So, by inequalities (2) and (3), we have

$$A - C \leq [f(d) - f(d-k)] - k[f(d+1) - f(d)],$$
$$B - D \geq [f(d(v_{d'+1}) + k) - f(d(v_{d'+1}))]$$
$$\qquad - k[f(d(v_{d'+1}) + k + 1) - f(d(v_{d'+1}) + k)].$$

Since $(f(x)-f(x-k))-k(f(x+1)-f(x))$ is an strictly increasing function and $d \leq a-1 < d(v_{d'+1})+k$, $A-C < B-D$. Thus by equality (1), $h(G) < h(G')$. ■

Theorem 3. *Let G' be a graph obtained by performing a proper accumulation in a K_aT graph G. Then $h(G') > h(G)$.*

Proof. Let $t_1, t_2, \ldots, t_k, t$, $k \geq 1$, be vertices in T of G such that

$$2 \leq d' = d(t_1) = d(t_2) = \cdots = d(t_k) \leq d(t) = d \leq a-k.$$

Let $V(K_a) = \{v_1, v_2, \ldots, v_a\}$ with $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_a)$, and G' be the resulting graph after the proper accumulation from $t_1, t_2, \ldots, t_k$ to t. Then

$$G' = G - t_1v_{d'} - t_2v_{d'} - \cdots - t_kv_{d'} + tv_{d+1} + tv_{d+2} + \cdots + tv_{d+k},$$

and G' is a K_aT graph from Lemma 3. Let

$$A = k[f(d') - f(d'-1)]; \qquad B = f(d(v_{d'})) - f(d(v_{d'})-k);$$
$$C = \sum_{i=1}^{k}[f(d(v_{d+i})+1) - f(d(v_{d+i}))]; \quad D = f(d+k) - f(d).$$

Clearly,

$$h(G) - h(G') = (A-D) - (C-B). \tag{4}$$

Since the accumulation is proper, there is no vertex of degree greater than $d'-1$ and less than $d+k$ in T of G'. By part (2) of Lemma 1, we have $d_{G'}(v_{d+k}) = d_{G'}(v_{d'})$, and then $d(v_{d+k}) = d(v_{d'}) - k - 1$ in G. Since $f(x+1) - f(x)$ is an increasing function and $d(v_{d+1}) \geq d(v_{d+2}) \geq \cdots \geq d(v_{d+k}) = d(v_{d'}) - k - 1$,

$$C \geq k[f(d(v_{d'})-k) - f(d(v_{d'})-k-1)]. \tag{5}$$

And by $d' \leq d$,

$$A \leq k[f(d) - f(d-1)]. \tag{6}$$

Thus by inequalities (5) and (6), we have

$$\begin{aligned}
A - D &\leq k[f(d) - f(d-1)] - [f(d+k) - f(d)];\\
C - B &\geq k[f(d(v_{d'}) - k) - f(d(v_{d'}) - k - 1)] - [f(d(v_{d'}))\\
&\quad - f(d(v_{d'}) - k)].
\end{aligned}$$

Since $k[f(x)-f(x-1)]-[f(x+k)-f(x)]$ is an strictly increasing function and $d \leq a-1 < d(v_{d'}) - k$, $A - D < C - B$, and so $h(G) < h(G')$ from equality (4). ■

References

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

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

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

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

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

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

[7] Y. Dong, S. Qiao, B. Chen, P. Wan, S. Zhang, Maximum values of degree-based entropies of bipartite graphs, *Appl. Math. Comput.* **401** (2021) 126094.

[8] M. Ghorbani, M. Dehmer, S. Zangi, Graph operations based on using distance-based graph entropies, *Appl. Math. Comput.* **333** (2018) 547–555.

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

[10] J. Yan, Topological structure of extremal graphs on the first degree-based graph entropies, *MATCH Commun. Math. Comput. Chem.* **85** (2021) 275–284.