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On the Minimality of Degree-Based Graph Entropy for Connected Graphs

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Abstract

Graph entropy quantifies uncertainty, characterizing both the efficiency of information extraction and the structural complexity of graphs. For diverse applications, numerous entropy measures have been defined based on distinct graph invariants. Determining the structural properties of minimum-entropy graphs is not only theoretically significant but also highly challenging. In this paper, by investigating two types of edge operations and their inverses, we improve and extend the existing conditions for reducing degree-based graph entropy. Our results provide a basis for developing a strategy to minimize the degree-based graph entropy of connected graphs with fixed numbers of vertices and edges.

1 Introduction

As an interdisciplinary concept, graph entropy primarily integrates theories and methods from information theory, graph theory, and applied mathematics, finding broad applications in chemistry, computational biology, network science, and computer science. Shannon's pioneering work [9] employed entropy to quantify the amount of information, and it has since served as a fundamental measure of disorder. In 1955, Rashevsky [8] first merged information theory with graph theory by introducing entropy to characterize the structural features of molecular graphs, enabling the estimation of their complexity and functional properties. Unlike the entropies proposed by Rashevsky [8] and Trucco [10], which are based on the number of vertices and edges respectively, Bonchev and Trinajstić [1] adopted distance as a graph invariant to address the problem of non-isomorphic graphs yielding identical entropy values. Their work formally introduced the concept of entropy into chemical graph theory, thus advancing research on various graph entropies. In 2008, Dehmer [4] defined the generalized graph entropy of a graph G as

$$I_f(G) = -\sum_{v\in S} \frac{f(v)}{\sum_{u\in S} f(u)} \log \frac{f(v)}{\sum_{u\in S} f(u)},$$

where f is a function from a given set S of elements of G to the set of positive real numbers, and the log has base 2. When f is assigned as the degree $d_G(v)$ of any vertex v in G, namely the number of vertices that v is adjacent to, we obtain the *degree-based graph entropy* [3]:

$$I_d(G) = -\sum_{v\in V(G)} \frac{d_G(v)}{\sum_{u\in V(G)} d_G(u)} \log \frac{d_G(v)}{\sum_{u\in V(G)} d_G(u)},$$

where $V(G)$ denotes the vertex set of G. Define $g(d_G(v)) = d_G(v)\log d_G(v)$ and let m be the edge number of G. Then an equivalent formula follows:

$$I_d(G) = \log(2m) - \frac{1}{2m} \sum_{v\in V(G)} g(d_G(v)). \tag{1}$$

Subsequent research has focused on investigating the extremal properties of I_d across diverse graph families. In [7], the minimum and maximum values of I_d for trees and cyclic graphs were derived, with the extremal graphs further characterized not only within these graph families but also in certain chemical graphs [3]. For bipartite graphs, Dong et al. determined the maximum values of I_d and identified the associated extremal graphs [5]. For general graphs, Yan [11] characterized the topological structures of connected graphs that achieve the minimum or maximum I_d, and proposed a conjecture regarding the minimum entropy of sparse graphs, which was later proven by Cambie and Mazzamurro in 2023 [2]. These findings indicate that determining the minimum properties of I_d in general graphs remains a challenging open problem. When graphs are allowed to be disconnected, Dong et al. [6] characterized the minimum-entropy graphs as those where each edge either belongs to a maximal clique, or lies between the maximal clique and a vertex not contained in the clique, with all other vertices being isolated. However, the structure of connected graphs with minimum I_d remains elusive to date. In [12], two types of edge operations were defined, together with conditions for reducing I_d. Later, Yan et al. proposed improved versions of these conditions and characterized the minimum-entropy graphs in connected dense graphs [13].

In this paper, we improve and extend the conditions for reducing degree-based graph entropy presented in [13] (see Theorems 2 and 4), while establishing conditions under which the inverses of the two edge operations from [12] reduce I_d (see Theorems 5 and 6). Our results provide potential tools for exploring the correlation between edge density and the minimality of degree-based graph entropy.

2 Preliminary definitions and results

In this paper, graphs will always be simple and connected. For a vertex v in a graph G, $N_G(v)$ denotes its neighbourhood, and $d_G(v) = |N_G(v)|$ for its degree. Where no confusion is likely, we will omit the subscript G.

A K_aT *graph* is a graph composed of two disjoint vertex sets, S and T, such that S is a clique with a vertices, T is an independent set, and for any vertices u, v in T, if $d(u) \geq d(v)$, then $N(v) \subseteq N(u)$. In [11], graphs with the minimum degree-based graph entropy were described as K_aT graphs.

For a K_aT graph G, given a and the degrees of all vertices in T, its structure is uniquely determined. Assuming that no vertex in T has degree exceeding $a-1$ (note that if a vertex has degree a, add it into S to form a larger clique), G can be formally denoted as $[1^{q_1}, 2^{q_2}, \ldots, (a-1)^{q_{a-1}}]_{K_a}$, where q_l is the number of the vertices in T with degree l for l from 1 to $a-1$. If $q_l = 0$, then l^{q_l} can be omitted from the sequence; if $q_l = 1$, the superscript q_l is redundant. Clearly, $\sum_{l=1}^{a-1} q_l = |T|$.

Let $S = \{v_1, v_2, \ldots, v_a\}$ with $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_a)$. By definition, every vertex in T with degree l is adjacent exclusively to $v_1, v_2, \ldots, v_l$. Thus, the neighborhood of the i-th vertex v_i in S includes all vertices in T with degree $\geq i$ (total count $\sum_{l=i}^{a-1} q_l$), and the other $a-1$ vertices in S, so $d(v_i) = a - 1 + \sum_{l=i}^{a-1} q_l$ for $1 \leq i \leq a-1$ and $d(v_a) = a - 1$.

To gain deeper insights into the structure of graphs with minimum I_d, two types of edge operations for K_aT graphs were proposed in [12]. We now introduce the first one. Let t and $s_1, s_2, \ldots, s_k$ be vertices in T with $d(t) = i$ and $d(s_1) = d(s_2) = \cdots = d(s_k) = j$, where $2 \leq k+1 \leq i \leq j$. A *k-edge distribution* from t to $s_1, s_2, \ldots, s_k$ is an operation that deletes edges $tv_i, tv_{i-1}, \ldots, tv_{i-k+1}$ and adds edges $s_1v_{j+1}, s_2v_{j+1}, \ldots, s_kv_{j+1}$. For brevity, it may occasionally be abbreviated as "a distribution". Figure 1 illustrates a 2-edge distribution in $[3^4]_{K_4}$.

Remark 1. If G' results from a k-edge distribution on G, then

$$G' = [1^{q_1}, 2^{q_2}, \ldots, (i-k)^{q_{i-k}+1}, \ldots, i^{q_i - 1}, \ldots, j^{q_j - k}, (j+1)^{q_{j+1}+k}, \ldots, (a-1)^{q_{a-1}}]_{K_a}.$$

Then degrees of vertices in S of G' are determined (note that the conclusion here also holds when $i = j$):

- $d_{G'}(v_p) = d_G(v_p) - 1 = a - 2 + \sum_{l=p}^{a-1} q_l$ for $p = i, i-1, \ldots, i-k+1$;
- $d_{G'}(v_{j+1}) = d_G(v_{j+1}) + k = a - 1 + k + \sum_{l=j+1}^{a-1} q_l$;
- others remain unchanged.

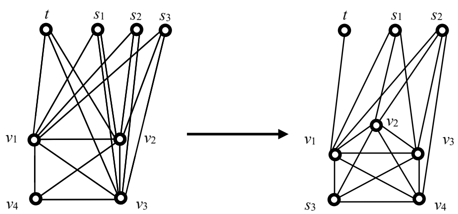

Figure 1. A distribution from t to s_2, s_3 in $[3^4]_{K_4}$.

The following theorem from [13] provides a condition for reducing the entropy I_d via a distribution.

Theorem 1. [13, Theorem 4] *Let* $G = [1^{q_1},2^{q_2},\ldots,(a-1)^{q_{a-1}}]_{K_a}$ *and* G' *be the graph obtained by a distribution from a vertex of degree* i *to* k *vertices of degree* j *in* G. *Then* $I_d(G) > I_d(G')$ *if*

$$\sum_{l=i-k+1}^{j} q_l \leq j - i + k + 1. \tag{2}$$

Straightforward calculations yield $I_d([3^4]_{K_4}) > I_d([1,3,4]_{K_5})$, but the distribution illustrated in Figure 1 fails the condition in Theorem 1, making our first main result, the following theorem, applicable here.

Theorem 2. *Let* $G = [1^{q_1},2^{q_2},\ldots,(a-1)^{q_{a-1}}]_{K_a}$ *and* G' *be the graph obtained by a distribution from a vertex of degree* i *to* k *vertices of degree* j *in* G. *Then* $I_d(G) \geq I_d(G')$ *if*

$$\left(i-j-k-1+\sum_{l=i-k+1}^{j} q_l\right)\left(i-\frac{k-1}{2}\right) \leq \left(j-i+\frac{k+1}{2}\right)\left(a-i+k-1+\sum_{l=j+1}^{a-1} q_l\right), \tag{3}$$

with $I_d(G) > I_d(G')$ *if the strict inequality in* (3) *holds.*

Recalling the assumption $2 \leq k+1 \leq i \leq j$ for the k-edge distribution, both the right-hand side of (3) and the factor $i - \frac{k-1}{2}$ on the left-hand side are positive. Consequently, (2) ensures that (3) holds strictly.

Remark 2. Theorem 2 improves and extends Theorem 1.

We next present the second edge operation introduced in [12]. Let $t_1, t_2, \ldots, t_k$ and s be vertices in T with $d(t_1) = d(t_2) = \cdots = d(t_k) = i$ and $d(s) = j$, where $2 \leq i \leq j \leq a - k$. A *$k$-edge accumulation* from $t_1, t_2, \ldots, t_k$ to s is an operation that deletes edges $t_1v_i, t_2v_i, \ldots, t_kv_i$ and adds edges $sv_{j+1}, sv_{j+2}, \ldots, sv_{j+k}$, also abbreviated as "an accumulation". Both the distribution and accumulation operations result in graphs that are still K_aT graphs [11], with the number of vertices and edges fixed. In Figure 2, $[2^4]_{K_4}$ is transformed into $[1^2, 2]_{K_5}$ via a 2-edge accumulation.

Remark 3. If G' results from a k-edge accumulation on G, then

$$G' = [1^{q_1},2^{q_2},\ldots,(i-1)^{q_{i-1}+k},i^{q_i-k},\ldots,j^{q_j-1},\ldots,(j+k)^{q_{j+k}+1},\ldots,(a-1)^{q_{a-1}}]_{K_a}.$$

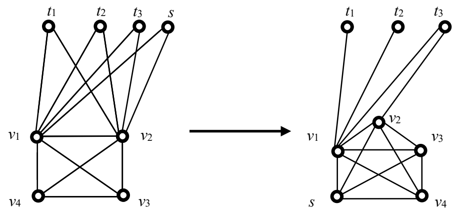

Figure 2. An accumulation from t_1, t_2 to s in $[2^4]_{K_4}$.

Then degrees of vertices in S of G' are determined:

- $d_{G'}(v_i) = d_G(v_i) - k = a - 1 - k + \sum_{l=i}^{a-1} q_l$;
- $d_{G'}(v_p) = d_G(v_p) + 1 = a + \sum_{l=p}^{a-1} q_l$ for $p = j+1, j+2, \ldots, j+k$;
- others remain unchanged.

A sufficient condition for reducing I_d through an accumulation, also from [13], is given as follows.

Theorem 3. [13, Theorem 5] *Let $G = [1^{q_1}, 2^{q_2}, \ldots, (a-1)^{q_{a-1}}]_{K_a}$ and G' be the graph obtained by an accumulation from k vertices of degree i to a vertex of degree j in G. Then $I_d(G) > I_d(G')$ if*

$$\sum_{l=i}^{j+k-1} q_l \leq j - i + k + 1. \tag{4}$$

Theorem 3 fails to support the fact that $I_d([2^4]_{K_4}) > I_d([1^2, 2]_{K_5})$ for the accumulation illustrated in Figure 2, whereas the following theorem, our second main result, suffices. For conciseness, we define a function as

$$\lambda(\alpha, \beta) = \left(\left(1 + \frac{\beta}{\alpha} \right)^{\frac{1}{\beta}} - 1 \right)^{-1},$$

where $\alpha > 0$ and $\beta \geq 1$.

Theorem 4. *Let $G = [1^{q_1}, 2^{q_2}, \ldots, (a-1)^{q_{a-1}}]_{K_a}$ and G' be the graph obtained by an accumulation from k vertices of degree i to a vertex of* *degree j in G. Then $I_d(G) \geq I_d(G')$ if*

$$\left(i - j - k - 1 + \sum_{l=i}^{j+k-1} q_l\right) i \leq (\lambda(j,k) - i + 1)\left(a - i + \sum_{l=j+k}^{a-1} q_l\right), \quad (5)$$

with $I_d(G) > I_d(G')$ if the strict inequality in (5) *holds.*

By Bernoulli's inequality, $\left(1+\frac{\beta}{\alpha}\right)^{\frac{1}{\beta}} \leq 1+\frac{1}{\alpha}$. Rearranging this inequality gives $\left(\left(1+\frac{\beta}{\alpha}\right)^{\frac{1}{\beta}} - 1\right)^{-1} \geq \alpha$, i.e., $\lambda(\alpha, \beta) \geq \alpha$, with equality if and only if $\beta = 1$. Consequently, the right-hand side of (5) is positive (note that $i \leq j \leq a-1$). It follows that under the assumption of (4), (5) must hold, meaning Theorem 3 is derivable from Theorem 4.

Remark 4. Theorem 4 improves and extends Theorem 3.

It is easy to see that the 1-edge distribution and 1-edge accumulation are identical, and when $k = 1$, (3) and (5) take the same form. Hence in this case, the conditions of Theorems 2 and 4 coincide, and the next corollary establishes this unified condition.

Corollary. *Let G' be the graph obtained by a distribution* (*or accumulation*) *from a vertex of degree i to a vertex of degree j in G. Then $I_d(G) \geq I_d(G')$ if*

$$\left(i - j - 2 + \sum_{l=i}^{j} q_l\right) i \leq (j - i + 1)\left(a - i + \sum_{l=j+1}^{a-1} q_l\right). \quad (6)$$

Let t and $s_1, s_2, \ldots, s_k$ be vertices in T such that $d(t) = i$ and $d(s_1) = d(s_2) = \cdots = d(s_k) = j$, where $i + k \leq j - 1$. A *k-edge inverse distribution* from $s_1, s_2, \ldots, s_k$ to t is the inverse of a k-edge distribution from t to $s_1, s_2, \ldots, s_k$: specifically, delete edges $s_1v_j, s_2v_j, \ldots, s_kv_j$ and add edges $tv_{i+1}, tv_{i+2}, \ldots, tv_{i+k}$.

Remark 5. If G' results from a k-edge inverse distribution on G, then

$$G' = [1^{q_1}, 2^{q_2}, \ldots, i^{q_i - 1}, \ldots, (i+k)^{q_{i+k}+1}, \ldots, (j-1)^{q_{j-1}+k}, j^{q_j - k}, \ldots, (a-1)^{q_{a-1}}]_{K_a}.$$

Then degrees of vertices in S of G' are determined:

- $d_{G'}(v_p) = d_G(v_p) + 1 = a + \sum_{l=p}^{a-1} q_l$ for $p = i+1, i+2, \ldots, i+k$;
- $d_{G'}(v_j) = d_G(v_j) - k = a - 1 - k + \sum_{l=j}^{a-1} q_l$;
- others remain unchanged.

Theorem 5 establishes a condition for reducing the entropy I_d via a k-edge inverse distribution, which is the third main result.

Theorem 5. *Let $G = [1^{q_1}, 2^{q_2}, \ldots, (a-1)^{q_{a-1}}]_{K_a}$ and G' be the graph obtained by an inverse distribution from k vertices of degree j to a vertex of degree i in G. Then $I_d(G) \geq I_d(G')$ if $\sum_{l=i+k}^{j-1} q_l \geq j - i - k - 1$, and*

$$\left(i-j+k+1+\sum_{l=i+k}^{j-1} q_l\right) \lambda(i,k) \geq (j-\lambda(i,k)-1)\left(a-i-k-1+\sum_{l=j}^{a-1} q_l\right), \quad (7)$$

with $I_d(G) > I_d(G')$ if the strict inequality in (7) holds.

Let $t_1, t_2, \ldots, t_k$ and s be vertices in T with $d(t_1) = d(t_2) = \cdots = d(t_k) = i$ and $d(s) = j$, where $i + 1 \leq j - k$. A *k-edge inverse accumulation* from s to $t_1, t_2, \ldots, t_k$ is the inverse of a k-edge accumulation from $t_1, t_2, \ldots, t_k$ to s: delete edges $sv_j, sv_{j-1}, \ldots, sv_{j-k+1}$ and add edges $t_1v_{i+1}, t_2v_{i+1}, \ldots, t_kv_{i+1}$.

Remark 6. If G' results from a k-edge inverse accumulation on G, then

$$G' = [1^{q_1}, 2^{q_2}, \ldots, i^{q_i-k}, (i+1)^{q_{i+1}+k}, \ldots, (j-k)^{q_{j-k}+1}, \ldots, j^{q_j-1}, \ldots, (a-1)^{q_{a-1}}]_{K_a}.$$

Then degrees of vertices in S of G' are determined:

- $d_{G'}(v_{i+1}) = d_G(v_{i+1}) + k = a - 1 + k + \sum_{l=i+1}^{a-1} q_l$;
- $d_{G'}(v_p) = d_G(v_p) - 1 = a - 2 + \sum_{l=p}^{a-1} q_l$ for $p = j, j-1, \ldots, j-k+1$;
- others remain unchanged.

Theorem 6, our final main result, presents a condition for reducing I_d through this operation.

Theorem 6. *Let $G = [1^{q_1}, 2^{q_2}, \ldots, (a-1)^{q_{a-1}}]_{K_a}$ and G' be the graph obtained by an inverse accumulation from a vertex of degree j to k vertices of degree i in G. Then $I_d(G) \geq I_d(G')$ if $\sum_{l=i+1}^{j-k} q_l \geq j - i - k - 1$, and*

$$\left(i-j+k+1+\sum_{l=i+1}^{j-k} q_l\right) i \geq \left(j-i-\frac{k+1}{2}\right)\left(a-i-2+\sum_{l=j-k+1}^{a-1} q_l\right), \quad (8)$$

with $I_d(G) > I_d(G')$ if the strict inequality in (8) *holds.*

When $k = 1$, (7) and (8) coincide in form, yielding the following condition for $I_d(G) \geq I_d(G')$.

Corollary. *Let G' be the graph obtained by an inverse distribution (or accumulation) from a vertex of degree j to a vertex of degree i in G. Then $I_d(G) \geq I_d(G')$ if $\sum_{l=i+1}^{j-1} q_l \geq j-i-2$, and*

$$\left(i-j+2+\sum_{l=i+1}^{j-1} q_l\right) i \geq (j-i-1)\left(a-i-2+\sum_{l=j}^{a-1} q_l\right). \tag{9}$$

Remark 7. We observe that the distribution and accumulation tend to form a larger clique, whereas their inverses tend to form a larger independent set. Furthermore, unlike Theorems 1 and 3, our conditions incorporate parameters characterizing the scales of the clique and the independent set, a feature that may prove useful for exploring the correlation between edge density and degree-based graph entropy minimality.

3 Proofs of main results

Lemma 1 provides a key inequality for the main results of this paper.

Lemma 1. *For an integer $k \geq 2$ and $x > k$,*

$$k\int_{x-\frac{k+1}{2}}^{x-\frac{k-1}{2}} \frac{1}{t}\,dt < \int_{x-k}^{x} \frac{1}{t}\,dt. \tag{10}$$

Proof. Let $\theta = \begin{cases} 1, & \text{if } k \text{ is odd;} \\ 0, & \text{if } k \text{ is even.} \end{cases}$ It is straightforward to verify that

$$\int_{x-k}^{x} \frac{1}{t}\,dt = \sum_{l=\frac{1}{2}(\theta+1)}^{\frac{1}{2}(k-1)} \left(\int_{x-\frac{k+1}{2}+l}^{x-\frac{k-1}{2}+l} \frac{1}{t}\,dt + \int_{x-\frac{k+1}{2}-l}^{x-\frac{k-1}{2}-l} \frac{1}{t}\,dt\right) + \theta\int_{x-\frac{k+1}{2}}^{x-\frac{k-1}{2}} \frac{1}{t}\,dt. \tag{11}$$

We claim that the function $\int_{x-1}^{x} \frac{1}{t}\,dt - \int_{x-l-1}^{x-l} \frac{1}{t}\,dt$ is strictly increasing on $(l+$

$1,+\infty)$ for $\frac{\theta+1}{2} \le l \le \frac{k-1}{2}$. This is evident as its derivative

$$\frac{1}{x} - \frac{1}{x-1} - \frac{1}{x-l} + \frac{1}{x-l-1} = \frac{l(2x-l-1)}{x(x-1)(x-l)(x-l-1)} > 0.$$

Since $x - \frac{k-1}{2} + l > x - \frac{k-1}{2} > l + 1$ (the latter inequality holds because $x > k$ and $l \le \frac{k-1}{2}$), by strict monotonicity, we have

$$\int_{x-\frac{k+1}{2}+l}^{x-\frac{k-1}{2}+l} \frac{1}{t}\,dt + \int_{x-\frac{k+1}{2}-l}^{x-\frac{k-1}{2}-l} \frac{1}{t}\,dt > 2\int_{x-\frac{k+1}{2}}^{x-\frac{k-1}{2}} \frac{1}{t}\,dt.$$

Substituting this into (11), we get

$$\int_{x-k}^{x} \frac{1}{t}\,dt > \frac{k-\theta}{2} \cdot 2\int_{x-\frac{k+1}{2}}^{x-\frac{k-1}{2}} \frac{1}{t}\,dt + \theta\int_{x-\frac{k+1}{2}}^{x-\frac{k-1}{2}} \frac{1}{t}\,dt = k\int_{x-\frac{k+1}{2}}^{x-\frac{k-1}{2}} \frac{1}{t}\,dt.$$

The proof is complete. ■

3.1 Proofs of Theorems 2 and 6

As the proofs of Theorems 2 and 6 rely on the identical lemmas, they are presented in a single subsection. Similarly, the proofs of Theorems 4 and 5 are grouped in the following subsection.

To prove Theorems 2 and 6, we need Lemma 3, whose proof depends on Lemma 2.

Lemma 2. *For an integer $k \ge 2$, the function*

$$f(x) = k\int_{x-\frac{k+1}{2}}^{x-\frac{k-1}{2}} \log t\,dt - \int_{x-k}^{x} \log t\,dt$$

is strictly decreasing on $(k,+\infty)$.

Proof. Computing the derivative, we obtain

$$\begin{aligned} f'(x) &= k\left(\log\left(x - \frac{k-1}{2}\right) - \log\left(x - \frac{k+1}{2}\right)\right) - (\log x - \log(x-k)) \\ &= k\int_{x-\frac{k+1}{2}}^{x-\frac{k-1}{2}} \frac{1}{t}\,dt - \int_{x-k}^{x} \frac{1}{t}\,dt < 0 \end{aligned}$$

by Lemma 1. Thus, $f(x)$ is strictly decreasing on $(k,+\infty)$ for $k \ge 2$. ■

Lemma 3. *For an integer k with $1 \le k < b < c$,*

$$\int_{b-k}^{b} \log t\, dt - \int_{c-k}^{c} \log t\, dt \le k \int_{b-\frac{k+1}{2}}^{b-\frac{k-1}{2}} \log t\, dt - k \int_{c-\frac{k+1}{2}}^{c-\frac{k-1}{2}} \log t\, dt,$$

with equality if and only if $k = 1$.

The proof follows immediately from Lemma 2 and is thus omitted.

Proof of Theorem 2. From (1) and Remark 1, we have

$$I_d(G) - I_d(G') = -\frac{1}{2m} \sum_{v \in V(G)} (g(d_G(v)) - g(d_{G'}(v))) = -\frac{1}{2m} \sum_{l=1}^{4} T_l, \quad (12)$$

where

$$T_1 = g(i) - g(i-k); \qquad T_2 = \sum_{p=i-k+1}^{i} \left(g\left(a-1+\sum_{l=p}^{a-1} q_l\right) - g\left(a-2+\sum_{l=p}^{a-1} q_l\right)\right);$$

$$T_3 = k\,(g(j) - g(j+1)); \quad T_4 = g\left(a-1+\sum_{l=j+1}^{a-1} q_l\right) - g\left(a-1+k+\sum_{l=j+1}^{a-1} q_l\right).$$

Since $g(x+\Delta) - g(x) = \int_x^{x+\Delta} \log t\, dt$, we derive

$$T_1 = \int_{i-k}^{i} \log t\, dt; \qquad T_2 = \sum_{p=i-k+1}^{i} \int_{a-2+\sum_{l=p}^{a-1} q_l}^{a-1+\sum_{l=p}^{a-1} q_l} \log t\, dt;$$

$$T_3 = -k \int_{j}^{j+1} \log t\, dt; \qquad T_4 = -\int_{a-1+\sum_{l=j+1}^{a-1} q_l}^{a-1+k+\sum_{l=j+1}^{a-1} q_l} \log t\, dt.$$

Clearly,

$$T_2 \le k \int_{a-2+\sum_{l=i-k+1}^{a-1} q_l}^{a-1+\sum_{l=i-k+1}^{a-1} q_l} \log t\, dt.$$

Thus, we obtain

$$\sum_{l=1}^{4} T_l \le \int_{i-k}^{i} \log t dt - \int_{a-1+\sum_{l=j+1}^{a-1} q_l}^{a-1+k+\sum_{l=j+1}^{a-1} q_l} \log t dt + k \int_{a-2+\sum_{l=i-k+1}^{a-1} q_l}^{a-1+\sum_{l=i-k+1}^{a-1} q_l} \log t dt - k \int_{j}^{j+1} \log t dt. \quad (13)$$

Since $k < i < a - 1 + k + \sum_{l=j+1}^{a-1} q_l$, by Lemma 3,

$$\int_{i-k}^{i} \log t\, dt - \int_{a-1+\sum_{l=j+1}^{a-1} q_l}^{a-1+k+\sum_{l=j+1}^{a-1} q_l} \log t\, dt \le k \int_{i-\frac{k+1}{2}}^{i-\frac{k-1}{2}} \log t\, dt - k \int_{a+\frac{k-3}{2}+\sum_{l=j+1}^{a-1} q_l}^{a+\frac{k-1}{2}+\sum_{l=j+1}^{a-1} q_l} \log t\, dt.$$

Substituting the above inequality into (13) and and dividing both sides by k, we get

$$\frac{1}{k}\sum_{l=1}^{4} T_l \le \int_{i-\frac{k+1}{2}}^{i-\frac{k-1}{2}} \log t dt - \int_{a+\frac{k-3}{2}+\sum_{l=j+1}^{a-1} q_l}^{a+\frac{k-1}{2}+\sum_{l=j+1}^{a-1} q_l} \log t dt + \int_{a-2+\sum_{l=i-k+1}^{a-1} q_l}^{a-1+\sum_{l=i-k+1}^{a-1} q_l} \log t dt - \int_{j}^{j+1} \log t dt. \quad (14)$$

The right-hand side of (14) can be rewritten as

$$\int_{i-\frac{k+1}{2}}^{i-\frac{k-1}{2}} \log \frac{t\left(t - i + \frac{k-3}{2} + a + \sum_{l=i-k+1}^{a-1} q_l\right)}{\left(t - i + k - 1 + a + \sum_{l=j+1}^{a-1} q_l\right)\left(t - i + j + \frac{k+1}{2}\right)}\, dt. \quad (15)$$

By (12), to prove $I_d(G) \ge I_d(G')$, it suffices to show $\sum_{l=1}^{4} T_l \le 0$. This requires the argument of the logarithm in (15) to be no greater than 1, which is equivalent to the following expression being nonpositive for all $t \in \left[i - \frac{k+1}{2}, i - \frac{k-1}{2}\right]$:

$$t\left(t-i+\frac{k-3}{2}+a+\sum_{l=i-k+1}^{a-1} q_l\right) - \left(t-i+k-1+a+\sum_{l=j+1}^{a-1} q_l\right)\left(t-i+j+\frac{k+1}{2}\right).$$

Simplifying the above yields:

$$\left(i-j-k-1+\sum_{l=i-k+1}^{j} q_l\right) t - \left(j-i+\frac{k+1}{2}\right)\left(a-i+k-1+\sum_{l=j+1}^{a-1} q_l\right). \quad (16)$$

We observe that $\left(j - i + \frac{k+1}{2}\right)\left(a - i + k - 1 + \sum_{l=j+1}^{a-1} q_l\right) > 0$. Thus, if $i - j - k - 1 + \sum_{l=i-k+1}^{j} q_l \le 0$, then (16)$< 0$, directly implying $I_d(G) > I_d(G')$.

Now suppose $i-j-k-1+\sum_{l=i-k+1}^{j} q_l > 0$. When t takes its maximum value $i-\frac{k-1}{2}$ in (16), we obtain

$$\left(i-j-k-1+\sum_{l=i-k+1}^{j} q_l\right)\left(i-\frac{k-1}{2}\right) - \left(j-i+\frac{k+1}{2}\right)\left(a-i+k-1+\sum_{l=j+1}^{a-1} q_l\right), \quad (17)$$

so (16)$\le$(17). By hypothesis (3), (17)≤ 0, whence $I_d(G) \ge I_d(G')$. In particular, if (17)< 0, then $I_d(G) > I_d(G')$ necessarily follows. This completes the proof. ■

Proof of Theorem 6. From Remark 6, $I_d(G) - I_d(G') = -\frac{1}{2m}\sum_{l=1}^{4} T_l$, where

$$T_1 = k\,(g(i) - g(i+1))\,; \qquad T_2 = \sum_{p=j-k+1}^{j}\left(g\left(a-1+\sum_{l=p}^{a-1} q_l\right) - g\left(a-2+\sum_{l=p}^{a-1} q_l\right)\right)\,;$$

$$T_3 = (g(j) - g(j-k))\,; \qquad T_4 = g\left(a-1+\sum_{l=i+1}^{a-1} q_l\right) - g\left(a-1+k+\sum_{l=i+1}^{a-1} q_l\right).$$

By an analogous argument to Theorem 2, we derive

$$\sum_{l=1}^{4} T_l \le \int_{j-k}^{j} \log t dt - \int_{a-1+\sum_{l=i+1}^{a-1} q_l}^{a-1+k+\sum_{l=i+1}^{a-1} q_l} \log t dt + k\int_{a-2+\sum_{l=j-k+1}^{a-1} q_l}^{a-1+\sum_{l=j-k+1}^{a-1} q_l} \log t dt - k\int_{i}^{i+1} \log t dt.$$

By Lemma 3,

$$\int_{j-k}^{j} \log t dt - \int_{a-1+\sum_{l=i+1}^{a-1} q_l}^{a-1+k+\sum_{l=i+1}^{a-1} q_l} \log t dt \le k\int_{j-\frac{k+1}{2}}^{j-\frac{k-1}{2}} \log t dt - k\int_{a+\frac{k-3}{2}+\sum_{l=i+1}^{a-1} q_l}^{a+\frac{k-1}{2}+\sum_{l=i+1}^{a-1} q_l} \log t dt.$$

Combining these results and dividing both sides by k, we get

$$\begin{aligned}\frac{1}{k}\sum_{l=1}^{4} T_l &\le \int_{j-\frac{k+1}{2}}^{j-\frac{k-1}{2}} \log t dt - \int_{a+\frac{k-3}{2}+\sum_{l=i+1}^{a-1} q_l}^{a+\frac{k-1}{2}+\sum_{l=i+1}^{a-1} q_l} \log t dt + \int_{a-2+\sum_{l=j-k+1}^{a-1} q_l}^{a-1+\sum_{l=j-k+1}^{a-1} q_l} \log t dt - \int_{i}^{i+1} \log t dt.\\ &= \int_{i}^{i+1} \log \frac{\left(t-i+j-\frac{k+1}{2}\right)\left(t-i+a-2+\sum_{l=j-k+1}^{a-1} q_l\right)}{t\left(t-i+a+\frac{k-3}{2}+\sum_{l=i+1}^{a-1} q_l\right)}\, dt.\end{aligned}$$

We proceed as in Theorem 2 to verify the integrand's argument is less than or equal to 1. Specifically,

$$\begin{aligned}&\left(t-i+j-\frac{k+1}{2}\right)\left(t-i+a-2+\sum_{l=j-k+1}^{a-1} q_l\right) - t\left(t-i+a+\frac{k-3}{2}+\sum_{l=i+1}^{a-1} q_l\right)\\ &= -\left(i-j+k+1+\sum_{l=i+1}^{j-k} q_l\right)t + \left(j-i-\frac{k+1}{2}\right)\left(a-i-2+\sum_{l=j-k+1}^{a-1} q_l\right)\\ &\le -\left(i-j+k+1+\sum_{l=i+1}^{j-k} q_l\right)i + \left(j-i-\frac{k+1}{2}\right)\left(a-i-2+\sum_{l=j-k+1}^{a-1} q_l\right)\end{aligned}$$

due to $\sum_{l=i+1}^{j-k} q_l \ge j-i-k-1$ and $t \ge i$. By hypothesis (8), the above expression is nonpositive. Thus, the integrand is nonpositive, which implies $I_d(G) \ge I_d(G')$ and equality fails if the strict inequality in (8) holds. The proof is complete. ■

3.2 Proofs of Theorems 4 and 5

The following lemma helps to derive the necessary inequality in Lemma 5.

Lemma 4. *For an integer $\beta \geq 2$ and $\alpha > 0$, the function*

$$f(x) = \beta \int_{x+\lambda(\alpha,\beta)-\alpha}^{x+\lambda(\alpha,\beta)-\alpha+1} \log t \, dt - \int_{x}^{x+\beta} \log t \, dt$$

is strictly increasing on $[\alpha, +\infty)$.

Proof. Let $h(x)$ denote the derivative of $f(x)$ for brevity. Then

$$h(x) = \beta \left(\log(x+\lambda(\alpha,\beta)-\alpha+1) - \log(x+\lambda(\alpha,\beta)-\alpha)\right) - \left(\log(x+\beta) - \log x\right).$$

Our aim is to prove $h(x) \geq 0$ for all $x \in [\alpha, +\infty)$, with equality if and only if $x = \alpha$. This is established through the following three claims:

Claim 1. $h(\alpha) = 0$.

Recall that $\lambda(\alpha, \beta) = \left(\left(1 + \frac{\beta}{\alpha}\right)^{\frac{1}{\beta}} - 1\right)^{-1}$. Then

$$\begin{aligned} h(\alpha) &= \beta \left(\log\left(\lambda(\alpha,\beta)+1\right) - \log \lambda(\alpha,\beta)\right) - \left(\log\left(\alpha+\beta\right) - \log \alpha\right) \\ &= \beta \log\left(1 + \frac{1}{\lambda(\alpha,\beta)}\right) - \log\left(1 + \frac{\beta}{\alpha}\right) \\ &= \beta \log\left(1 + \frac{\beta}{\alpha}\right)^{\frac{1}{\beta}} - \log\left(1 + \frac{\beta}{\alpha}\right) \\ &= 0, \end{aligned}$$

which completes the proof of Claim 1.

Claim 2. $\lim_{x \to +\infty} h(x) = 0$.

Using logarithm properties, rewrite $h(x)$ as:

$$h(x) = \log\left(\left(1 + \frac{1}{x+\lambda(\alpha,\beta)-\alpha}\right)^{\beta} \cdot \left(1 - \frac{\beta}{x+\beta}\right)\right).$$

As $x \to +\infty$, the fractional terms tend to 0, so the argument tends to 1. Thus, $\lim_{x \to +\infty} h(x) = 0$, proving Claim 2.

Claim 3. There exists some η such that $h(x)$ is strictly increasing for $x < \eta$ and strictly decreasing for $x \geq \eta$.

To analyze the monotonicity of $h(x)$, we compute its derivative

$$h'(x) = \beta\frac{(2\lambda(\alpha,\beta)-2\alpha-\beta+1)x+(\lambda(\alpha,\beta)-\alpha)(\lambda(\alpha,\beta)-\alpha+1)}{x(x+\beta)(x+\lambda(\alpha,\beta)-\alpha)(x+\lambda(\alpha,\beta)-\alpha+1)}. \tag{18}$$

First, We show $2\lambda(\alpha,\beta) - 2\alpha - \beta + 1 < 0$. By the definition of $\lambda(\alpha,\beta)$, this is equivalent to proving

$$\left(1 + \frac{2}{2\alpha+\beta-1}\right)^{\beta} < 1 + \frac{\beta}{\alpha}. \tag{19}$$

For $\alpha > 0$ and $\beta \geq 2$, substituting $x = \alpha + \beta$ and $k = \beta$ into (10), Lemma 1 yields

$$\beta \int_{\alpha+\frac{\beta-1}{2}}^{\alpha+\frac{\beta+1}{2}} \frac{1}{t}\, dt < \int_{\alpha}^{\alpha+\beta} \frac{1}{t}\, dt.$$

Integrating $\frac{1}{t}$ gives the logarithmic form

$$\beta \left(\log\left(\alpha + \frac{\beta+1}{2}\right) - \log\left(\alpha + \frac{\beta-1}{2}\right)\right) < \log\left(\alpha+\beta\right) - \log\alpha,$$

which simplifies to

$$\log\left(1 + \frac{2}{2\alpha+\beta-1}\right)^{\beta} < \log\left(1 + \frac{\beta}{\alpha}\right).$$

As log is strictly increasing, (19) follows, so $2\lambda(\alpha,\beta) - 2\alpha - \beta + 1 < 0$.

From Section 2, we know $\lambda(\alpha,\beta) > \alpha$, so both the denominator of $h'(x)$ in (18) and the constant term $\left(\lambda\left(\alpha,\beta\right) - \alpha\right)\left(\lambda(\alpha,\beta) - \alpha + 1\right)$ are positive. Given the negative coefficient of x in the numerator (proven above), $h'(x)$ has a unique real root:

$$\eta = -\frac{\left(\lambda(\alpha,\beta) - \alpha\right)\left(\lambda(\alpha,\beta) - \alpha + 1\right)}{2\lambda(\alpha,\beta) - 2\alpha - \beta + 1},$$

with $h'(x) > 0$ for $x < \eta$, $h'(\eta) = 0$, and $h'(x) < 0$ for $x > \eta$. This completes the proof of Claim 3.

Combining Claims 1-3: $h(x)$ is strictly increasing from 0 to $h(\eta)$ on $[\alpha,\eta)$ and strictly decreasing from $h(\eta)$ to 0 as $x\to+\infty$ on $[\eta,+\infty)$. Thus, $h(x)=0$ if and only if $x=\alpha$. Since $f'(x)=h(x)\geq 0$ with equality holding at exactly one point, $f(x)$ is strictly increasing on $[\alpha,+\infty)$. The proof is complete. ∎

Note that $\lambda(\alpha,1)=\alpha$, so Lemma 5 follows directly from Lemma 4.

Lemma 5. *For an integer $\beta\geq 1$ and $\alpha>0$ with $\alpha\leq b<c$, we have*

$$\int_c^{c+\beta}\log t dt-\int_b^{b+\beta}\log t dt\leq\beta\int_{c+\lambda(\alpha,\beta)-\alpha}^{c+\lambda(\alpha,\beta)-\alpha+1}\log t dt-\beta\int_{b+\lambda(\alpha,\beta)-\alpha}^{b+\lambda(\alpha,\beta)-\alpha+1}\log t dt,$$

with equality if and only if $\beta=1$.

Proof of Theorem 4. By Remark 3, $I_d(G)-I_d(G')=-\frac{1}{2m}\sum_{l=1}^{4}T_l$, where

$$T_1=g(j)-g(j+k);\qquad T_2=\sum_{p=j+1}^{j+k}\left(g\left(a-1+\sum_{l=p}^{a-1}q_l\right)-g\left(a+\sum_{l=p}^{a-1}q_l\right)\right);$$

$$T_3=k\left(g(i)-g(i-1)\right);\qquad T_4=g\left(a-1+\sum_{l=i}^{a-1}q_l\right)-g\left(a-1-k+\sum_{l=i}^{a-1}q_l\right).$$

Using the same reasoning as in preceding theorems,

$$\sum_{l=1}^{4}T_l\leq\int_{a-1-k+\sum_{l=i}^{a-1}q_l}^{a-1+\sum_{l=i}^{a-1}q_l}\log t\,dt-\int_j^{j+k}\log t\,dt+k\int_{i-1}^{i}\log t\,dt-k\int_{a-1+\sum_{l=j+k}^{a-1}q_l}^{a+\sum_{l=j+k}^{a-1}q_l}\log t\,dt.$$

Since $j<a-1-k+\sum_{l=i}^{a-1}q_l$, Lemma 5 implies

$$\int_{a-1-k+\sum_{l=i}^{a-1}q_l}^{a-1+\sum_{l=i}^{a-1}q_l}\log t\,dt-\int_j^{j+k}\log t\,dt\leq k\int_{a-k-j-1+\lambda(j,k)+\sum_{l=i}^{a-1}q_l}^{a-k-j+\lambda(j,k)+\sum_{l=i}^{a-1}q_l}\log t\,dt-k\int_{\lambda(j,k)}^{\lambda(j,k)+1}\log t\,dt.$$

Thus,

$$\begin{aligned}\frac{1}{k}\sum_{l=1}^{4}T_l&\leq\int_{a-k-j-1+\lambda(j,k)+\sum_{l=i}^{a-1}q_l}^{a-k-j+\lambda(j,k)+\sum_{l=i}^{a-1}q_l}\log t dt-\int_{\lambda(j,k)}^{\lambda(j,k)+1}\log t dt+\int_{i-1}^{i}\log t dt-\int_{a-1+\sum_{l=j+k}^{a-1}q_l}^{a+\sum_{l=j+k}^{a-1}q_l}\log t dt\\&=\int_{i-1}^{i}\log\frac{t\left(t-i+a-k-j+\lambda(j,k)+\sum_{l=i}^{a-1}q_l\right)}{(t-i+1+\lambda(j,k))\left(t-i+a+\sum_{l=j+k}^{a-1}q_l\right)}\,dt.\end{aligned}$$

For $i-1 \leq t \leq i$, direct computation gives

$$t\left(t-i+a-k-j+\lambda(j,k)+\sum_{l=i}^{a-1} q_l\right)-(t-i+1+\lambda(j,k))\left(t-i+a+\sum_{l=j+k}^{a-1} q_l\right)$$
$$=\left(i-j-k-1+\sum_{l=i}^{j+k-1} q_l\right)t-(\lambda(j,k)-i+1)\left(a-i+\sum_{l=j+k}^{a-1} q_l\right).$$

Since $\lambda(j,k) \geq j \geq i$, the constant term is positive. If $i-j-k-1+\sum_{l=i}^{j+k-1} q_l \leq 0$, then $I_d(G) > I_d(G')$. If the coefficient is positive, substituting $t=i$ and using hypothesis (5), we have the inequality

$$(i-j-k-1+\sum_{l=i}^{j+k-1} q_l)i-(\lambda(j,k)-i+1)(a-i+\sum_{l=j+k}^{a-1} q_l) \leq 0.$$

Following the reasoning from prior theorems, we conclude $I_d(G) \geq I_d(G')$, with $I_d(G) < I_d(G')$ if the strict inequality in (5) holds. The proof is complete. ■

Proof of Theorem 5. By Remark 5, $I_d(G)-I_d(G') = -\frac{1}{2m}\sum_{l=1}^{4} T_l$, where

$$T_1 = g(i)-g(i+k); \qquad T_2 = \sum_{p=i+1}^{i+k}\left(g\left(a-1+\sum_{l=p}^{a-1} q_l\right)-g\left(a+\sum_{l=p}^{a-1} q_l\right)\right);$$

$$T_3 = k\left(g(j)-g(j-1)\right); \qquad T_4 = g\left(a-1+\sum_{l=j}^{a-1} q_l\right)-g\left(a-1-k+\sum_{l=j}^{a-1} q_l\right).$$

$$\sum_{l=1}^{4} T_l \leq \int_{a-1-k+\sum_{l=j}^{a-1} q_l}^{a-1+\sum_{l=j}^{a-1} q_l} \log t\,dt-\int_{i}^{i+k} \log t\,dt+k\int_{j-1}^{j} \log t\,dt-k\int_{a-1+\sum_{l=i+k}^{a-1} q_l}^{a+\sum_{l=i+k}^{a-1} q_l} \log t\,dt.$$

Since $i < a-k-1+\sum_{l=j}^{a-1} q_l$, Lemma 5 further implies

$$\int_{a-1-k+\sum_{l=j}^{a-1} q_l}^{a-1+\sum_{l=j}^{a-1} q_l} \log t dt-\int_{i}^{i+k} \log t dt \leq k\int_{a-k-i-1+\lambda(i,k)+\sum_{l=j}^{a-1} q_l}^{a-k-i+\lambda(i,k)+\sum_{l=j}^{a-1} q_l} \log t dt-k\int_{\lambda(i,k)}^{\lambda(i,k)+1} \log t dt.$$

As always, we get

$$\frac{1}{k}\sum_{l=1}^{4} T_l \leq \int_{a-k-i-1+\lambda(i,k)+\sum_{l=j}^{a-1} q_l}^{a-k-i+\lambda(i,k)+\sum_{l=j}^{a-1} q_l} \log t\, dt - \int_{\lambda(i,k)}^{\lambda(i,k)+1} \log t\, dt + \int_{j-1}^{j} \log t\, dt - \int_{a-1+\sum_{l=i+k}^{a-1} q_l}^{a+\sum_{l=i+k}^{a-1} q_l} \log t\, dt$$
$$= \int_{\lambda(i,k)}^{\lambda(i,k)+1} \log \frac{\left(t-1+a-k-i+\sum_{l=j}^{a-1} q_l\right)\left(t-\lambda(i,k)-1+j\right)}{t\left(t-\lambda(i,k)-1+a+\sum_{l=i+k}^{a-1} q_l\right)}\, dt.$$

From the hypothesis $j-i-k-1 \leq \sum_{l=i+k}^{j-1} q_l$, together with $t \geq \lambda(i,k)$, we deduce

$$\left(t-1+a-k-i+\sum_{l=j}^{a-1} q_l\right)\left(t-\lambda(i,k)-1+j\right) - t\left(t-\lambda(i,k)-1+a+\sum_{l=i+k}^{a-1} q_l\right)$$
$$= -\left(i-j+k+1+\sum_{l=i+k}^{j-1} q_l\right)t + \left(j-\lambda(i,k-1)\right)\left(a-i-k-1+\sum_{l=j}^{a-1} q_l\right)$$
$$\leq -\left(i-j+k+1+\sum_{l=i+k}^{j-1} q_l\right)\lambda(i,k) + \left(j-\lambda(i,k)-1\right)\left(a-i-k-1+\sum_{l=j}^{a-1} q_l\right).$$

By hypothesis (7), the above expression is nonpositive. Following the same reasoning, we complete the proof. ■

References

[1] D. Bonchev, N. Trinajstić, Information theory, distance matrix, and molecular branching, *Chem. Phys.* **67** (1977) 4517–4533.

[2] S. Cambie, M. Mazzamurro, Resolution of Yan's conjecture on entropy of graphs, *MATCH Commun. Math. Comput. Chem.* **89** (2023) 389–404.

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

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

[5] 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.

[6] Y. Dong, M. Gadouleau, P. Wan, S. Zhang, Graphs with minimum degree-entropy, *Inf. Sci.* **671** (2024) #120629.

[7] A. Ghalavand, M. Eliasi, A. R. Ashrafi, First degree-based entropy of graphs, *J. Appl. Math. Comput.* **59** (2019) 37–46.

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

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

[10] E. Trucco, A note on the information content of graphs, *Bull. Math. Biophys.* **18** (1956) 129–135.

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

[12] J. Yan, F. Guan, Graph operations decreasing values of degree-based graph entropies, *MATCH Commun. Math. Comput. Chem.* **89** (2023) 405–414.

[13] J. Yan, F. Guan, Minimal degree-based graph entropy for dense graphs, *MATCH Commun. Math. Comput. Chem.* **94** (2025) 687–699.