

# Resolution of Yan’s Conjecture on Entropy of Graphs

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## Abstract

The first degree-based entropy of a graph is the Shannon entropy of its degree sequence normalized by the degree sum. In this paper, we characterize the connected graphs with given order  $n$  and size  $m$  that minimize the first degree-based entropy whenever  $n - 1 \leq m \leq 2n - 3$ , thus extending and proving a conjecture by Yan.

## 1 Introduction

The Shannon entropy of graph invariants has attracted significant attention in mathematical chemistry as a measure of uniformity of a molecular structural aspect of interest. Mowshowitz [16] discussed the entropy of the cardinality of the vertex orbits under graph automorphisms, while Bonchev [1] focused on the entropy of the cardinality of the subset of vertices having the same degree or eccentricity. Dehmer [7] introduced a

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more general framework to study the Shannon entropy of any graph invariant, normalized by its sum to yield an information functional. This approach was subsequently applied in [9] to compare the properties of real and synthetic chemical structures. Although Shannon entropy is conceptually and computationally simple, its careful and context-informed normalisation and interpretation pose some challenges, as they require knowing the range of values the measure can take. Finding the measure's extremal value for graphs satisfying natural constraints is essential for this aim. This question of determining the extremal properties of the Shannon entropy for a graph invariant was first posed by Dehmer and Kraus in [8]. They remarked on the complexity of the problem, which depends on the presence of structural constraints on the graph.

A graph invariant of particular interest in mathematical chemistry is given by the powers  $d^c$  of vertex degrees  $d$ , also in light of its connection to the first Zagreb index [10]. Cao et al. [3] raised the question of finding extremal values of the Shannon entropy for the first degree-based entropy, that is, for the case  $c = 1$ . They proved extremal properties for certain classes of graphs, including trees, unicyclic, bicyclic and chemical graphs of given order and size. In [4], they provided numerical results for the case  $c \neq 1$ , as well as bounds depending on the smallest and largest degree of the graph. Lu et al. [14, 15] also used the smallest and largest degree and Jensen's inequality to prove bounds on the entropy of degree powers. The relation between the entropy and different values of the degree power  $c$  was explored by [5], who proved numerical results for trees, unicyclic, bipartite and triangle-free graphs with a small number of vertices. Ilić [13] proved that the path graph maximizes the degree-based entropy among trees. Ghalavand et al. [11] used the Strong Mixing Variable method to prove maximality results for trees, unicyclic and bicyclic graphs.

In [2], we determined the minimum first degree-based entropy among all graphs with a given size, showing that the extremal graphs are precisely the colex graphs. In this paper, we do so for connected graphs with given size  $m$  and order  $n$ , which we call  $(n, m)$ -graphs, for the case when  $n - 1 \leq m \leq 2m - 3$ . This problem was first presented by Yan [19], who solved it when  $n - 1 \leq m \leq n + 5$  and conjectured that the degree sequence of the

graph that minimises the first-degree based graph entropy when  $m \geq n+9$  is  $(n-1, m-n+2, 2^{m-n+1}, 1^{2n-m-3})$ . Note that the cases  $n-1 \leq m \leq n+1$  correspond to trees, unicyclic, and bicyclic graphs, solved in [3]. Here we refine Yan's conjecture, first of all by noticing that the proposed degree sequence is only possible when  $m \leq 2n-3$ , and then showing that the conjecture holds in the wider range  $n+6 \leq m \leq 2n-3$ . This extends the characterization of the minimal first degree-based entropy to the range  $n-1 \leq m \leq 2n-3$ . The extremal graphs, i.e. the graphs minimizing the entropy among all  $(n, m)$ -graphs, are presented in Table 1. Except for a few cases, they are the same as in [18], which solves the same problem in the case that  $f$  is a function for which both  $f$  and its derivative  $f'$  are convex (which is not the case for  $f(x) = x \log(x)$ ).

Let us now start by formally defining the measure of interest. Here the logarithm will always denote the base 2 logarithm. Remark, however, that analogous arguments hold for the natural logarithm.

**Definition 1.** The first degree-based entropy of a graph  $G$  with degree sequence  $(d_i)_{1 \leq i \leq n}$  and size  $m$  equals

$$I(G) = - \sum_{i=1}^n \frac{d_i}{2m} \log \left( \frac{d_i}{2m} \right).$$

If we let  $f(x) = x \log(x)$  and  $h(G) = \sum_i f(d_i) = \sum_i d_i \log(d_i)$ , then we have  $I(G) = \log(2m) - \frac{1}{2m} h(G)$ . Thus, determining the minimum of  $I(G)$  is equivalent to determining the maximum of  $h(G)$ .

By [19, Theorem 4], we know that the graph maximizing  $h(G)$  among all  $(n, m)$ -graphs is a threshold graph. This implies in particular that it has a universal vertex  $v$ , i.e. a vertex adjacent to all other vertices and hence with degree  $n-1$ . Now, the graph  $G \setminus v$ , obtained by removing  $v$  and all its incident edges from  $G$ , is a  $(n-1, m-n+1)$ -graph. Taking into account that  $d_G(u) = d_{G \setminus v}(u) + 1$  for every vertex  $u \neq v$ , we note that it is sufficient to find the  $(n-1, m-n+1)$ -graph maximizing  $h_1(G)$ , where  $h_1(G)$  is formed by taking into account that the original degrees are larger by one. We extend this idea towards the setting where there are  $c$  universal vertices initially. Then, we compute the extremal graphs maximizing the

$m = n - 1 + a$ $0 \leq a \leq n - 2$ $a \notin \{3, 5, 6\}$	
$m = n + 2$	
$m = n + 4$	
$m = n + 5$	

**Table 1.** Overview of extremal  $(n, m)$ -graphs minimizing the entropy. Compare to [19, Table 1] and [3, Theorems 1,2, and 3]

related function  $h_c(G)$  given only the size (and fixed large order essentially,

as explained in Subsection 1.1). We do so by induction. In Section 2 we compute some extremal graphs for small size. These are the base cases for the induction. Then by taking a vertex of minimum degree and relating  $h_c(G)$  with  $h_c(G \setminus v)$ , we perform the induction in Section 3. Besides a few exceptions, the extremal graphs turn out to be the star, contrary to the extremal graphs for  $h(G)$  when only the graph size is given, for which the extremal graphs are colex graphs, see [2]. The precise statement is formulated in Theorem 1. At the end of the section, in Subsection 3.1, we apply Theorem 1 to characterize the graphs minimizing the entropy among  $(n, m)$ -graphs when  $n - 1 \leq m \leq 2n - 3$ , thus proving an extended version of the conjecture formulated by Yan [19, Conj. 6].

The main ideas of the proof are given in Section 3. Some necessary tools and computations are gathered in Subsection 1.1 and Section 4.

## 1.1 Definitions and notation

In this paper, we will express the entropy in terms of other functions and use help functions in the computations. These are defined here.

**Definition 2.** For any constant  $c \geq 0$ , we define the function  $f_c(x) = (x + c) \cdot \log(x + c)$ . For a graph  $G$  with degree sequence  $(d_i)_{1 \leq i \leq n}$ , we define  $h_c(G) = \sum_i f_c(d_i)$ . When  $c = 0$ , we just write  $h(G)$  for  $h_0(G) = \sum_i d_i \log(d_i)$ .

When  $c \geq 2$ , the function  $h_c(G)$  depends on the number of vertices as well, since isolated vertices contribute  $f_c(0) = c \log c > 0$ . Thus, we will compare graphs with a different order by extending the order, i.e. adding isolated vertices in such a way that the graphs have the same order. If the orders of two graphs to be compared were  $N$  and  $n$ , with  $N \geq n$ , we could have defined  $h_c^N(G) = \sum_i f_c(d_i) + (N - n)f_c(0)$  and used  $h_c^N$  for the comparison, but we preferred to keep the notation light.

We remark here that it will be sufficient to focus on connected graphs.

*Remark.* When omitting the isolated vertices, the graph maximizing  $h_c(G)$  among all graphs of size  $m$  is a connected graph. For this, note that identifying two vertices in different components with strictly positive degrees

$d_u, d_v$  leads to an increase of the value  $h_c(G)$  since  $f_c$  is a strictly convex function, i.e.  $f_c(d_u + d_v) + f_c(0) > f_c(d_u) + f_c(d_v)$ .

In some proofs, we will also make use of the following function.

**Definition 3.** The function  $\Delta_c$  is defined by  $\Delta_c(x) = f_c(x) - f_c(x - 1) = \log(e) + \int_{x+c-1}^{x+c} \log t \, dt$ .

Note that  $\Delta_c$  is a strictly concave, increasing function.

Throughout the paper, we will use the following notation:  $S_k$ ,  $P_k$ , and  $K_k$  denote respectively the star, the path, and the complete graph with  $k$  vertices, and  $K_k^-$  is  $K_k$  with one edge removed.

## 2 Extremal graphs for small size

In this section, we compute the extremal graphs maximizing  $h_1(G)$  for  $m \leq 10$  and for  $h_c(G)$  with  $c \geq 2$  for  $m \leq 6$ .

**Lemma 1.** For  $m \leq 10$ , among all graphs with  $m$  edges,  $h_1(G)$  is maximized by

$$G = \begin{cases} S_{m+1} & \text{if } m \notin \{3, 5, 6\} \\ K_3 & \text{if } m = 3 \\ K_4^- \text{ and } S_6 & \text{if } m = 5 \\ K_4 & \text{if } m = 6. \end{cases}$$

*Proof.* A computer program can verify this claim<sup>†</sup>. Since  $h_1(G)$  only depends on the degree sequence of the graph, for a given  $m \leq 10$ , it is enough to list all degree sequences of graphs of size  $m$  and then compute  $h_1$  for each sequence. To list all degree sequences, it is sufficient to list all integer partitions of  $2m$  and then to establish which of these are valid degree sequences using one of several existing criteria (see, e.g., [17]). For example, one can use the function `parts()` from the R-package `partitions` [12] to list all partitions of  $2m$  and check which ones are degree sequences using `is_graphical()` from the R-package `igraph` [6]. ■

<sup>†</sup>[https://github.com/MatteoMazzamurro/extrema-graph-entropy/blob/main/minimal\\_entropy\\_small\\_size.R](https://github.com/MatteoMazzamurro/extrema-graph-entropy/blob/main/minimal_entropy_small_size.R)

**Lemma 2.** For  $c \geq 2$  and  $m \leq 6$ , among all graphs with  $m$  edges,  $h_c(G)$  is maximized by

$$G = \begin{cases} S_{m+1} & \text{if } m \neq 3 \\ K_3 & \text{if } m = 3. \end{cases}$$

Remark that in this Lemma, one has to take into account isolated vertices when comparing graphs with different order.

*Proof.* For  $m \in \{1, 2\}$  nothing needs to be done, as there is only one connected graph of size  $m$ . When  $m = 3$ , there are precisely 3 connected graphs and we observe that

$$\begin{aligned} h_c(P_4) = 2f_c(1) + 2f_c(2) &< h_c(S_4) = 3f_c(1) + f_c(3) \\ &< h_c(K_3) = 3f_c(2) + f_c(0). \end{aligned}$$

The first inequality is true due to the strict convexity of the function  $f_c$ . The second inequality is true since  $\Delta_c$  (Definition 3) is strictly concave and thus  $\Delta_c(3) + \Delta_c(1) < 2\Delta_c(2)$ .

By the inequality of Karamata, it is sufficient to consider the degree sequences of graphs with size  $m$  that are not majorized by the degree sequences of other such graphs. With a simple computer program<sup>‡</sup>, we verify those.

For  $m = 4$ , these non-majorized degree sequences are

$$\vec{v}_1^4 = \{4, 1, 1, 1, 1\} \text{ and } \vec{v}_2^4 = \{3, 2, 2, 1, 0\}.$$

For  $m = 5$ , they are

$$\vec{v}_1^5 = \{5, 1, 1, 1, 1, 1\}, \vec{v}_2^5 = \{4, 2, 2, 1, 1, 0\}, \text{ and } \vec{v}_3^5 = \{3, 3, 2, 2, 0, 0\}.$$

For  $m = 6$ , the sequences are

$$\vec{v}_1^6 = \{6, 1, 1, 1, 1, 1, 1\}, \vec{v}_2^6 = \{5, 2, 2, 1, 1, 1, 0\},$$

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<sup>‡</sup>[https://github.com/StijnCambie/EntropyGraphs/blob/main/ExtrG\\_h\\_c\\_for\\_smallm.py](https://github.com/StijnCambie/EntropyGraphs/blob/main/ExtrG_h_c_for_smallm.py)

$$\vec{v}_3^6 = \{4, 3, 2, 2, 1, 0, 0\}, \text{ and } \vec{v}_4^6 = \{3, 3, 3, 3, 0, 0, 0\}.$$

Now we verify that  $h_c(\vec{d}) = \sum_i f_c(d_i)$  is always maximized by the first degree sequence.

For  $4 \leq m \leq 6$ , we have

$$\begin{aligned} h_c(\vec{v}_1^m) - h_c(\vec{v}_2^m) &= \Delta_c(m) + \Delta_c(1) - 2\Delta_c(2) \\ &\geq \int_{c-1}^c \log\left(\frac{(t+1)(t+4)}{(t+2)^2}\right) dt > 0, \end{aligned}$$

the last inequality is true since  $(t+1)(t+4) > (t+2)^2$  whenever  $t \geq 1$ .

For  $m \in \{5, 6\}$  we analogously have

$$\begin{aligned} h_c(\vec{v}_1^m) - h_c(\vec{v}_3^m) &= \Delta_c(m) + \Delta_c(m-1) + 2\Delta_c(1) - \Delta_c(3) - 3\Delta_c(2) \\ &\geq \int_{c-1}^c \log\left(\frac{(t+5)(t+4)(t+1)^2}{(t+3)(t+2)^3}\right) dt \\ &> 0. \end{aligned}$$

The last inequality being true since  $(t+5)(t+4)(t+1)^2 > (t+3)(t+2)^3$  whenever  $t \geq 1$ .

For the final case, we have

$$\begin{aligned} h_c(\vec{v}_1^6) - h_c(\vec{v}_4^6) &= \Delta_c(6) + \Delta_c(5) + \Delta_c(4) + 3\Delta_c(1) - 3\Delta_c(3) - 3\Delta_c(2) \\ &= \int_{c-1}^c \log\left(\frac{(t+6)(t+5)(t+4)(t+1)^3}{(t+3)^3(t+2)^3}\right) dt \\ &> 0. \end{aligned}$$

When  $c = 2$ , this can be computed<sup>§</sup>. For  $c \geq 3$ , this is due to

$$(t+6)(t+5)(t+4)(t+1)^3 > (t+3)^3(t+2)^3$$

for  $t \geq 2$ . Finally, it is also clear that the extremal degree sequences do correspond to the star  $S_{m+1}$ . ■

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<sup>§</sup>It is approximately 0.0908



### 3 Graphs maximizing $h_c(G)$ given the size

In this section, we prove the following theorem that gives the precise characterization of extremal graphs for  $h_c(G)$  where  $c \geq 1$  is an integer (for  $c = 0$ , this was done in [2]).

**Theorem 1.** *Among all graphs with  $m$  edges,  $h_1(G)$  is maximized by*

$$G = \begin{cases} S_{m+1} & \text{if } m \notin \{3, 5, 6\} \\ K_3 & \text{if } m = 3 \\ K_4^- \text{ and } S_6 & \text{if } m = 5 \\ K_4 & \text{if } m = 6. \end{cases}$$

For any  $c \geq 2$ , among all graphs with  $m$  edges and  $n > m$  vertices,  $h_c(G)$  is maximized by

$$G = \begin{cases} S_{m+1} & \text{if } m \neq 3 \\ K_3 & \text{if } m = 3. \end{cases}$$

*Proof.* Assume we know the extremal graphs with size at most  $m - 1$ . By Lemmas 1 and 2, this has been done for  $m \leq 6$  and  $m \leq 10$  when  $c = 1$ . So we assume  $m \geq 7$ , and even  $m \geq 11$  if  $c = 1$ . Let  $G$  be an extremal graph with size  $m$  for which the minimum (non-zero) degree is equal to  $b$ . The latter implies that there are at least  $b + 1$  vertices with degree at least  $b$  and thus  $m \geq \binom{b+1}{2}$ . Let  $v$  be a vertex with degree  $b$  and let  $d_1, d_2, \dots, d_b$  be the degrees of the neighbours of  $v$ .

If  $b = 1$ , we have

$$\begin{aligned} h_c(G) &= h_c(G \setminus v) + f_c(1) - f_c(0) + \Delta_c(d_1) \\ &\leq h_c(S_m) + f_c(1) - f_c(0) + \Delta_c(m) \\ &= h_c(S_{m+1}) \end{aligned}$$

and equality occurs if and only if  $G = S_{m+1}$ .

Now assume  $b \geq 2$ . Note that  $\sum_{i=1}^b d_i \leq m + \binom{b}{2}$  by the analog of the handshaking lemma since every edge which is not part of the subgraph  $G[N(v)]$  induced by the neighbours of  $v$  can be counted at most once.

Since  $\Delta_c$  is strictly concave, we have

$$\begin{aligned} h_c(G) - h_c(G \setminus v) &= f_c(b) - f_c(0) + \sum_{i=1}^b \Delta_c(d_i) \\ &\leq f_c(b) - f_c(0) + b \cdot \Delta_c\left(\frac{m + \binom{b}{2}}{b}\right) \\ &:= LHS(m, b, c). \end{aligned}$$

On the other hand, we also have

$$\begin{aligned} h_c(S_{m+1}) - h_c(S_{m-b+1}) &= f_c(m) - f_c(m-b) + b\Delta_c(1) \\ &:= RHS(m, b, c). \end{aligned}$$

By computations performed in Section 4, we know that the first is smaller than the second, i.e.  $LHS(m, b, c) < RHS(m, b, c)$ . Hence

$$h_c(G) < h_c(S_{m+1}) - h_c(S_{m-b+1}) + h_c(G \setminus v).$$

Now,  $G \setminus v$  has  $m - b$  edges, here  $m - b \geq 4$  (for  $c \geq 2$ ) and  $m - b \geq 7$  (for  $c = 1$ ). Due to Lemmas 1 and 2, we have  $h_c(G \setminus v) \leq h_c(S_{m-b+1})$ . Therefore we conclude that  $h_c(G) < h_c(S_{m+1})$ .

By complete induction, we have the whole characterization. ■

### 3.1 Proof of Yan's Conjecture

We now prove an extended version of Yan's conjecture [19, Conj.6].

**Theorem 2.** *When  $n - 1 \leq m \leq 2n - 3$ , the extremal  $(n, m)$ -graph mini-*

mizing the entropy has a degree sequence of the form

$$\left\{ \begin{array}{ll} (n-1, m-n+2, 2^{m-n+1}, 1^{2n-m-3}) & \text{if } 2n-3 \geq m \geq n+6 \\ & \text{or } m \in \{n, n+1, n+3\}, \\ (n-1, 4^4, 1^{n-5}) & \text{if } m = n+5, \\ (n-1, 4^2, 3^2, 1^{n-5}) \text{ or } (n-1, 6, 2^5, 1^{n-7}) & \text{if } m = n+4, \\ (n-1, 3^3, 1^{n-4}) & \text{if } m = n+2, \\ (n-1, 1^{n-1}) & \text{if } m = n-1. \end{array} \right.$$

These graphs are presented in Table 1.

In other words, when  $n \leq m \leq 2n-3$ , the extremal  $(n, m)$ -graph minimizing the entropy is such that, deleting its universal vertex, one obtains the  $(n-1, m-n+1)$ -graph  $G$  maximizing  $h_1(G)$ , as described in Theorem 1.

*Proof of Theorem 2.* By [19, Theorem 4], we know the extremal  $(n, m)$ -graph is a threshold graph. This implies in particular that it has a universal vertex  $v$  with degree  $n-1$ . Now  $G' = G \setminus v$  is a  $(n-1, m-n+1)$ -graph. Taking into account that  $d_G(u) = d_{G'}(u) + 1$  for every vertex  $u \neq v$ , we note that

$$h(G) = f(n-1) + h_1(G').$$

Now since  $m-n+1 \leq n-2$ , we note that the extremal structure for  $G'$  is determined in Theorem 1 and the conclusion is immediate.  $\blacksquare$

## 4 Computational lemmas

In this section, we prove that

$$LHS(m, b, c) = f_c(b) - f_c(0) + b \cdot \left( f_c \left( \frac{m + \binom{b}{2}}{b} \right) - f_c \left( \frac{m + \binom{b}{2}}{b} - 1 \right) \right)$$

and

$$RHS(m, b, c) = f_c(m) - f_c(m-b) + b \cdot (f_c(1) - f_c(0))$$

satisfy  $LHS(m, b, c) < RHS(m, b, c)$  for every  $b \geq 2$  and  $m \geq \binom{b+1}{2}$  whenever  $m \geq 7$  and  $c \geq 1$ , or  $m \geq 4$  and  $c \geq 2$ .

We do this by means of the following lemmas. In Lemma 3, we show that for fixed  $b$  and  $c$ , it is sufficient to prove the inequality for the smallest  $m$  in the range. After that, we prove it in the cases for which  $m = \binom{b+1}{2}$  in Lemma 4 and for the remaining cases in Lemma 5.

The proofs are mainly computational and there are alternative computations that lead to the same conclusion  $\blacksquare$ .

**Lemma 3.** *Fix  $b \geq 2$  and  $c \geq 1$ . Then  $RHS(m, b, c) - LHS(m, b, c)$  is an increasing function in  $m$ .*

*Proof.* We want to prove that the derivative of this quantity with respect to  $m$  is positive. To compute the derivative, taking into account the chain rule and  $\frac{d}{dx} f_c(x) = \log(x + c) + \log(e)$ , we have that

$$\begin{aligned} & \frac{d}{dm} (RHS(m, b, c) - LHS(m, b, c)) \\ &= \log\left(\frac{m+c}{m-b+c}\right) - \log\left(\frac{m+\binom{b}{2}+bc}{m+\binom{b}{2}+bc-b}\right) > 0. \end{aligned}$$

The inequality now follows the fact that whenever  $0 < b < y < z$ , we have  $\frac{y}{y-b} > \frac{z}{z-b}$ . Here it is enough to take  $y = m + c$  and  $z = m + \binom{b}{2} + bc$ .  $\blacksquare$

**Lemma 4.** *Fix  $b \geq 2$  and  $c \geq 1$ . Let*

$$LL(b, c) = (b+1)f_c(b) - f_c(0) - bf_c(b-1)$$

and

$$RL(b, c) = f_c\left(\binom{b+1}{2}\right) - f_c\left(\binom{b}{2}\right) + b \cdot (f_c(1) - f_c(0)).$$

Then

$$LL(b, c) < RL(b, c)$$

if  $c = 1$  and  $b \geq 4$ , or  $c \geq 2$  and  $b \geq 3$ .

$\blacksquare$ See, for example, <https://arxiv.org/abs/2205.03357> for an alternative proof of Lemma 4

*Proof.* The cases  $1 \leq c \leq 3$  can be verified directly using the formulae: solving numerically the resulting inequalities in the variable  $b$ , one finds that the inequality holds as long as  $b > 3.24$ ,  $b > 2.53$ , and  $b > 2.35$  for  $c = 1$ ,  $c = 2$ , and  $c = 3$ , respectively<sup>¶</sup>.

For  $c \geq 4$  and  $b \geq 3$ , write

$$\begin{aligned} RL(b, c) &= f_c \left( \binom{b}{2} + b \right) - f_c \left( \binom{b}{2} \right) + b\Delta_c(1) \\ &= \sum_{i=1}^b \left[ f_c \left( \binom{b}{2} + i \right) - f_c \left( \binom{b}{2} + i - 1 \right) \right] + b\Delta_c(1) \\ &= \sum_{i=1}^b \Delta_c \left( \binom{b}{2} + i \right) + b\Delta_c(1), \end{aligned}$$

and

$$\begin{aligned} LL(b, c) &= b(f_c(b) - f_c(b-1)) + f_c(b) - f_c(0) \\ &= b\Delta_c(b) + f_c(b) - f_c(0) \\ &= b\Delta_c(b) + \sum_{i=1}^b [f_c(i) - f_c(i-1)] \\ &= b\Delta_c(b) + \sum_{i=1}^b \Delta_c(i). \end{aligned}$$

Then

$$\begin{aligned} RL(b, c) - LL(b, c) &= \sum_{i=1}^b \left[ \Delta_c \left( \binom{b}{2} + i \right) - \Delta_c(i) \right] - b(\Delta_c(b) - \Delta_c(1)) \\ &> b \left[ \Delta_c \left( \binom{b}{2} + b \right) - \Delta_c(b) \right] - b(\Delta_c(b) - \Delta_c(1)) \\ &= b \left[ \Delta_c \left( \binom{b+1}{2} \right) + \Delta_c(1) - 2\Delta_c(b) \right] \end{aligned} \tag{1}$$

where inequality (1) follows from  $b \geq 2$  and the strict concavity of  $\Delta_c(x)$ .

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<sup>¶</sup>[https://github.com/MatteoMazzamurro/extrema-graph-entropy/blob/main/lemma\\_4\\_base\\_cases.R](https://github.com/MatteoMazzamurro/extrema-graph-entropy/blob/main/lemma_4_base_cases.R)

Then, by definition 3,

$$\begin{aligned}
 & RL(b, c) - LL(b, c) \\
 & \geq b \int_{c-1}^c \left[ \log \left( t + \binom{b+1}{2} \right) + \log(t+1) - 2\log(t+b) \right] dt
 \end{aligned}$$

For the integral to be positive, it is enough that, for  $c-1 < t < c$ ,

$$\left( t + \binom{b+1}{2} \right) (t+1) - (t+b)^2 > 0,$$

which is equivalent to

$$t(b-2)(b-1) > b(b-1). \tag{2}$$

Now, since  $b \geq 3$ , inequality (2) holds if and only if  $t > \frac{b}{b-2}$ . Furthermore,  $b \geq 3$  also implies  $\frac{b}{b-2} \leq 3$ . But  $c \geq 4$  so  $t > c-1 = 3 \geq \frac{b}{b-2}$ . Therefore  $RL(b, c) > LL(b, c)$  for  $c \geq 4$  and  $b \geq 3$  as well. ■

**Lemma 5.** *It is true that  $LHS(7, 3, 1) < RHS(7, 3, 1)$  and  $LHS(7, 2, 1) < RHS(7, 2, 1)$ . For any  $c \geq 2$ , it is true that  $LHS(4, 2, c) < RHS(4, 2, c)$ .*

*Proof.* By direct computation,  $RHS(7, 3, 1) - LHS(7, 3, 1) \approx 0.26$  and  $RHS(7, 2, 1) - LHS(7, 2, 1) \approx 0.52$  and thus  $LHS(7, 3, 1) < RHS(7, 3, 1)$ , and  $LHS(7, 2, 1) < RHS(7, 2, 1)$ .  $LHS(4, 2, c) < RHS(4, 2, c)$  is equivalent to

$$2\Delta_c(2.5) + \Delta_c(2) < \Delta_c(4) + \Delta_c(3) + \Delta_c(1).$$

This is true for every  $c \geq 2$  since

$$\int_{c-1}^c \log \left( \left( t + \frac{5}{2} \right)^2 (t+2) \right) dt < \int_{c-1}^c \log ((t+4)(t+3)(t+1)) dt,$$

as  $(t + \frac{5}{2})^2 (t+2) < (t+4)(t+3)(t+1)$  for every  $t \geq 1$ . ■

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