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 first-degree based graph entropy and the Shannon entropy of other graph invariants have attracted significant attention in organic chemistry, as measures of uniformity of a graph’s structural aspect of interest [7, 11, 5]. Although Shannon entropy is conceptually and computationally simple, its careful and context-informed normalisation and interpretation poses some challenges. Determining the range of values the Shannon entropy of a graph invariant can take is a non-trivial task as it may depend on the presence of structural constraints on the graph [4]. Solving this issue requires first and foremost the identification of the measure’s extremal values for graphs satisfying natural constraints.

In [2], we determined the minimum first degree-based entropy among all graphs with a given size. Here 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 $n - 1 \leq m \leq 2n - 3$. This problem was first presented by Yan [9], who conjectured that the degree sequence of the graph minimising the first-degree based graph entropy when $m \geq n + 9$ is $(n - 1, m - n + 2, 2^{m-n+1}, 1^{2n-m-3})$. Here we refine this conjecture, first of all by noticing that such degree sequence is only possible when $m \leq 2n - 3$, and then showing how, with some adjustments, the conjecture can be extended to the range $n - 1 \leq m \leq 2n - 3$. We finally proceed to prove it. The extremal graphs, i.e. the graphs minimizing the entropy among all $(n, m)$-graphs, are presented in Table 1.

Let us now start by formally defining the measure of interest. Here the logarithm will always denote 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 $h(G)$.

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

\[ m = n + 2 \]

\[ m = n + 4 \]

\[ m = n + 5 \]

| Table 1: Overview of extremal \((n, m)\)-graphs minimizing the entropy |
|---------------------------------------------------------------|
| \begin{align*}
  n - 2 - a & \quad a \\
  \end{align*} |
| \begin{align*}
  n - 4 \\
  \end{align*} |
| \begin{align*}
  n - 5 & \quad n - 7 \\
  \end{align*} |
| \begin{align*}
  n - 5 \\
  \end{align*} |

By [9, Theorem 4], we know that the graph maximizing \(h(G)\) among all \((n, m)\)-graphs is a threshold graph. This implies in particular that the graph has a universal vertex \(v\) with degree \(n - 1\). Now \(G \setminus v\) is a \((m - n + 1, n - 1)\)-graph. Taking into account that \(d_G(u) = d_{G \setminus v}(u) + 1\) for every vertex \(u \in V \setminus v\), we note that it is sufficient to find the \((m - n + 1, n - 1)\)-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 related function \(h_c(G)\) given only the size (and fixed large order essentially, as explained in Subsection [11]). We do so by induction. In Section 2 we compute the 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 7. At the end of the
section, in Subsection 3.1 we apply Theorem 7 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 [6], 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

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 \(h(G) = \sum d_i \log(d_i)\).

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. add isolated vertices in such a way that the graphs have the same order. We could have defined \(h_c(G) = \sum f_c(d_i) + (N - n)f_c(0)\) to do so, but preferred to keep the notation light.

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

Observation 3. 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 4. The function \(\Delta_c\) is defined by \(\Delta_c(x) = f_c(x) - f_c(x - 1) = 1 + f_{x+c} - \int_{x+c-1}^{x} \log t \, dt\).

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

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 5. For \(m \leq 10\), among all graphs with \(m\) edges, we have that \(h_1(G)\) is maximized by

\[
G = \begin{cases} 
K_{1,m} = S_{m+1} & \text{if } m \notin \{3, 4, 6\} \\
K_3 & \text{if } m = 3 \\
K_4^- = C(5, 3) \text{ and } S_6 & \text{if } m = 5 \\
K_4 & \text{if } m = 6.
\end{cases}
\]

Proof. A computer program can verify this claim. 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 establish which of these are valid degree sequences using one of several existing criteria (see, e.g., [5]). For example, one can use the function \texttt{parts()} from the R-package \texttt{partitions} [6] to list all partitions of \(2m\) and check which ones are degree sequences using \texttt{is\_graphical()} from the R-package \texttt{igraph} [3] (see Appendix A). \(\square\)

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

\[
G = \begin{cases} 
K_{1,m} & \text{if } m \neq 3 \\
K_3 & \text{if } m = 3.
\end{cases}
\]
Here 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

$$h_c(P_4) = 2f_c(1) + 2f_c(2) < h_c(S_4) = 3f_c(1) + f_c(3) < h_c(K_3) = 3f_c(2) + f_c(0).$$

The first inequality is true due to the strict convexity of the function $f_c$. The second inequality is true since $\Delta_c$ (Definition 1) 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, we verify those.

For $m = 4$ and $m = 5$, these non-majorized degree sequences are respectively $v_4^1 = \{4, 1, 1, 1\}, v_4^2 = \{3, 2, 2, 1, 0\}$ and $v_5^1 = \{5, 1, 1, 1, 1\}, v_5^2 = \{4, 2, 2, 1, 1, 0\}, v_5^3 = \{3, 3, 2, 2, 0, 0\}$. For $m = 6$, these degree sequences are $v_6^1 = \{6, 1, 1, 1, 1, 1\}, v_6^2 = \{5, 2, 2, 1, 1, 0\}, v_6^3 = \{4, 3, 2, 2, 1, 0, 0\}, v_6^4 = \{3, 3, 3, 3, 0, 0, 0\}$.

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

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

$$h_c\left(\mathcal{d}_1\right) - h_c\left(\mathcal{d}_2\right) = \Delta_c(m) + \Delta_c(1) - 2\Delta_c(2) \geq \int_{c-1}^c \log ((t+1)(t+4)) - \log ((t+2)^2) \, dt > 0.$$

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

$$h_c\left(\mathcal{d}_1\right) - h_c\left(\mathcal{d}_3\right) = \Delta_c(m) + \Delta_c(m-1) + 2\Delta_c(1) - \Delta_c(3) - 3\Delta_c(2)$$

$$\geq \int_{c-1}^c \log ((t+5)(t+4)(t+1)^2) - \log ((t+3)(t+2)^3) \, dt > 0.$$

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

$$h_c\left(\mathcal{d}_1\right) - h_c\left(\mathcal{d}_4\right) = \Delta_c(6) + \Delta_c(5) + \Delta_c(4) + 3\Delta_c(1) - 3\Delta_c(3) - 3\Delta_c(2)$$

$$= \int_{c-1}^c \log ((t+6)(t+5)(t+4)(t+1)^3) - \log ((t+3)^3(t+2)^3) \, dt > 0.$$

When $c = 2$, this can be computed. 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 with the star $S_{m+1} = K_1,m$.

\[\square\]

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]).

\[1\]https://github.com/StijnCambie/EntropyGraphs/blob/main/ExtrG_h_c_forsmallm.py
\[2\]It is approximately 0.0629
**Theorem 7.** Among all graphs with m edges, we have that \( h_1(G) \) is maximized by

\[
G = \begin{cases} 
K_{1,m} = S_{m+1} & \text{if } m \not\in \{3, 4, 6\} \\
K_3 & \text{if } m = 3 \\
K_4^- = C(5, 3) \text{ and } S_6 & \text{if } m = 5 \\
K_4 & \text{if } m = 6.
\end{cases}
\]

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

\[
G = \begin{cases} 
K_{1,m} & \text{if } m \neq 3 \\
K_3 & \text{if } m = 3.
\end{cases}
\]

**Proof.** Assume we know the extremal graphs with size at most \( m - 1 \). By Lemmas 5 and 6 this has been done for \( m \leq 6 \) and for \( m \leq 10 \) 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 \( d_1, d_2, \ldots, d_b \) be the degrees of the neighbours of \( v \).

If \( b = 1 \), we have

\[
h_c(G) = h_c(G \setminus v) + f_c(1) - f_c(0) + \Delta_c(d_1) 
\leq h_c(K_{1,m-1}) + f_c(1) - f_c(0) + \Delta_c(m) 
= h_c(K_{1,m})
\]

and equality occurs if and only if \( G = K_{1,m} \).

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 \( G \backslash N(v) \) can be counted at most once. Since \( \Delta_c \) is strictly concave, we have

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

On the other hand, we also have

\[
h_c(K_{1,m}) - h_c(K_{1,m-b}) = f_c(m) - f_c(m-b) + b\Delta_c(1) 
:= RHS(m, b, c).
\]

By computations performed in Section 4 we know that the first is smaller than the second, i.e. \( LHS(m, b, c) < RHS(m, b, c) \). 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 5 and 6 we have \( h_c(G \setminus v) \leq h_c(K_{1,m-b}) \).

So we conclude that

\[
h_c(G) = h_c(G \setminus v) + f_c(b) - f_c(0) + \sum_{i=1}^b \Delta_c(d_i) 
\leq h_c(G \setminus v) + f_c(b) - f_c(0) + b \cdot \Delta_c\left(\frac{m + \binom{b}{2}}{b}\right) 
\leq h_c(K_{1,m-b}) + f_c(m) - f_c(m-b) + b\Delta_c(1) 
= h_c(K_{1,m}).
\]

By complete induction, we have the whole characterization. \( \square \)
3.1 Proof of Yan’s Conjecture

We now prove an extended version of Yan’s conjecture [9, Conj.6].

**Theorem 8.** 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 \(G\) described in Theorem [7] for the \( c = 1 \) case, i.e. the graph with \( m' = m - n + 1 \) edges maximizing \( h_1(G) \). That is, the extremal \((n,m)\)-graph has degree sequence

\[
\begin{align*}
(n - 1, m - n + 2) &\quad \text{if } 2n - 3 \geq m \geq n + 6 \text{ or } m \in \{n, n + 1, n + 3\}, \\
(n - 1, 4^{n-5}) &\quad \text{if } m = n + 5, \\
(n - 1, 4^2, 3^2, 1^{n-5}) or (n - 1, 6, 2^5, 1^{n-7}) &\quad \text{if } m = n + 4, \\
(n - 1, 3^3, 1^{n-4}) &\quad \text{if } m = n + 2, \\
(n - 1, 1^{n-1}) &\quad \text{if } m = n - 1.
\end{align*}
\]

These graphs are presented in Table [7].

**Proof.** By [9, Theorem 4], we know that 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 \((m - n + 1, n - 1)\)-graph. Taking into account that \( d_G(u) = d_{G'}(u) + 1 \) for every vertex \( u \in V\setminus v \), 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 [7] and the conclusion is immediate. \( \square \)

4 Computational claims

In this section, we prove that

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

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 claims. In Claim [9] we prove that for fixed \( b \) and \( c \), it is sufficient to prove it for the smallest \( m \) in the range. After that, it is proven in the cases for which \( m = \binom{b+1}{2} \) in Claim [10] and for the remaining cases in Claim [11].

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

**Claim 9.** 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 \( \frac{d}{dx} f_c(x) = \log(x + c) + 1 \), we have that

\[
\frac{d}{dm} (RHS(m, b, c) - LHS(m, b, c)) = \log \left( \frac{m + c}{m - b + c} \right) - \log \left( \frac{m + \binom{b}{2} + bc}{m + \binom{b}{2} + bc - b} \right) > 0.
\]

The inequality now follows the fact 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 \( z = m + \binom{b}{2} + bc \). \( \diamond \)
Claim 10. 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 $b \geq 3$.

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 $b > 2.34$ for $c = 1$, $c = 2$, and $c = 3$, respectively. A proof that $RL(b, c) - LL(b, c)$ is increasing in $b$, has been put in Appendix B, where an alternative strategy for the verification of this claim has been given.

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

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

$$= \sum_{i=1}^{b} \left[ f_c\left(\binom{b}{2} + i\right) - f_c\left(\binom{b}{2} + i - 1\right) \right] + b\Delta_c(1)$$

$$= \sum_{i=1}^{b} \Delta_c\left(\binom{b}{2} + i\right) + b\Delta_c(1),$$

and

$$LL(b, c) = b \left( f_c(b) - f_c(b - 1) \right) + f_c(b) - f_c(0)$$

$$= b\Delta_c(b) + f_c(b) - f_c(0)$$

$$= b\Delta_c(b) + \sum_{i=1}^{b} \left[ f_c(i) - f_c(i - 1) \right]$$

$$= b\Delta_c(b) + \sum_{i=1}^{b} \Delta_c(i).$$

Then

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

$$> b \left[ \Delta_c\left(\binom{b}{2} + b\right) - \Delta_c(b) \right] - b \left( \Delta_c(b) - \Delta_c(1) \right)$$

$$= b \left[ \Delta_c\left(\binom{b+1}{2}\right) + \Delta_c(1) - 2\Delta_c(b) \right]$$

where inequality (1) follows from $b \geq 2$ and the strict concavity of $\Delta_c(x)$. Then, by definition 4

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

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
\[ t(b - 2)(b - 1) > b(b - 1). \]  
(2)

Now, since \( b \geq 3 \), inequality (2) holds if and only if \( t > \frac{b}{b - 2} \). Furthermore, \( b \geq 3 \) also implies \( \frac{b}{b - 2} < 3 \). 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.

\[ \text{Claim 11. It is true that } LHS(7, 3, 1) < RHS(7, 3, 1) \text{ and } LHS(7, 2, 1) < RHS(7, 2, 1). \]

For any \( c \geq 2 \), it is true that \( LHS(4, 2, c) < RHS(4, 2, c) \).

**Proof.** The values \( RHS(7, 3, 1) - LHS(7, 3, 1) \) and \( RHS(7, 2, 1) - LHS(7, 2, 1) \) are approximately 0.18 and 0.36 respectively and thus \( LHS(7, 3, 1) < RHS(7, 3, 1) \) and \( LHS(7, 2, 1) < RHS(7, 2, 1) \). The second inequality is equivalent to
\[ \Delta_c(4) + \Delta_c(3) + \Delta_c(1) > 2\Delta_c(2) + \Delta_c(2). \]

This is true for every \( c \geq 2 \) since
\[ \int_{c-1}^{c} \log ((t+4)(t+3)(t+1)) \, dt > \int_{c-1}^{c} \log \left( \left(\frac{t+5}{2}\right)^2 \right) \, dt, \]
as \( (t+4)(t+3)(t+1) > \left(\frac{t+5}{2}\right)^2 \) \( (t+2) \) for every \( t \geq 1 \). \[\Box\]

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A Codes

The following R code can be used to prove Lemma 5.

```r
# load necessary packages
library(partitions)
library(igraph)

# define function h_c
h_c <- function(x,c){
    # avoid issues with log(0)
    if(c==0){
        x[x==0] <- 1
    }
    ans <- sum((x+c)*log(x+c))
    return(ans)
}

# allow tolerance in the comparison to account for machine precision
tol<-1e-6

# initialize empty list of degree sequences
h_c_max <- list()

for(m in 3:10){
    # find partitions of 2m
    parts_m <- as.matrix(parts(2*m))
    # select partitions that are valid degree sequences
    is_graphical_m <- apply(parts_m,MARGIN=2,is_graphical)
    graphical_parts_m <- as.matrix(parts_m[,is_graphical_m])
    # find which degree sequence(s) maximize(s) h_c
    h_c_m <- apply(graphical_parts_m,MARGIN=2,h_c,c=1)
    h_c_m_max <- graphical_parts_m[,which((max(h_c_m)-h_c_m)<tol)]
    # add the degree sequence(s) maximizing h_c_m to the list
    h_c_max <- append(h_c_max,list(h_c_m_max))
}
```

B Precise verification of Claim 10

For easy reference, we restate Claim 10 here.

**Claim 12.** 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 \(b \geq 3\).
Proof. We first prove that the derivative of this quantity with respect to $b$ is positive. We have

$$\frac{d}{db} RL(b, c) = \frac{2b+1}{2} \left( \log \left( \left( \frac{b+1}{2} \right) + c \right) + 1 \right) - \frac{2b-1}{2} \left( \log \left( \left( \frac{b}{2} \right) + c \right) + 1 \right) + f_e(1) - f_e(0)$$

$$\frac{d}{db} LL(b, c) = (b+1) (\log(b+c) + 1) - b (\log(b+c) + 1) + f_e(b) - f_e(b-1)$$

Combining these two expressions, we can write

$$\frac{d}{db} (RL(b, c) - LL(b, c)) = J_1(b, c) + J_2(b, c) + J_3(b, c),$$

where

$$J_1(b, c) = \frac{2b-1}{2} \left( \log \left( \left( \frac{b+1}{2} \right) + c \right) - \log \left( \left( \frac{b}{2} \right) + c \right) - 2 \log(b+c) + 2 \log(b+c-1) \right),$$

$$J_2(b, c) = c (\log(c+1) - \log(c) - \log(b+c) + \log(b+c-1)), $$

$$J_3(b, c) = \log \left( \left( \frac{b+1}{2} \right) + c \right) + \log(c+1) - 2 \log(b+c).$$

It is sufficient to prove that $J_i(b, c) \geq 0$ for $i \in \{1, 2, 3\}$ for the above conditions on $b$ and $c$.

By expanding the binomial coefficient, we rewrite $J_1(b, c)$ as

$$J_1(b, c) = \frac{2b-1}{2} \log \left( \frac{(b^2 + b + 2c)(b+c-1)^2}{(b^2 - b + 2c)(b+c)^2} \right).$$

Then $J_1(b, c) > 0$ if and only if $g(b, c) > 0$, where

$$g(b, c) = (b^2 + b + 2c)(b+c-1)^2 - (b^2 - b + 2c)(b+c)^2.$$ 

This can be simplified as

$$g(b, c) = 2(b-3)bc + 2(b-2)c^2 + b + 2c - b^2.$$ 

Hence we can see that, whenever $b \geq 3$,

$$\frac{\partial}{\partial c} g(b, c) = 4(b-2)c + 2(b-3)b + 2 > 0,$$

and so $g(b, c)$ is a strictly increasing function in $c$ whenever $b \geq 3$.

For $c = 1$ we have that $g(b, 1) = b^2 - 3b - 2 > 0$ for $b \geq 4$. Similarly, for $c = 2$, we get $g(b, 2) = 3b^2 - 3b - 12 > 0$ for $b \geq 3$. Thus $g(b, c) > 0$ (and hence $J_1(b, c) > 0$) for $c = 1$ and $b \geq 4$, and for $c \geq 2$ and $b \geq 3$.

Analogous arguments apply to $J_2$ and $J_3$.

$J_2(b, c) > 0$ since $\log \left( 1 + \frac{1}{b} \right) > \log \left( 1 + \frac{1}{b+c-1} \right)$ when $b-1 > 0$.

For $J_3(b, c)$ note that

$$2 \left( \left( \frac{b+1}{2} \right) + c \right) (c+1) - 2(b+c)^2 = (bc - 2c - b)(b-1),$$

which is non-negative whenever $b, c \geq 3$.

Combining these results and substituting in equation (B), we have $\frac{d}{db} (RL(b, c) - LL(b, c)) > 0$ for $c \geq 3$. 
For the remaining cases, consider the sum $J_2(b, c) + J_3(b, c)$. When $c = 1$,

$$J_2(b, 1) + J_3(b, 1) = \log \left( \frac{2b(b^2 + b + 2)}{(b + 1)^3} \right).$$

Now,

$$2b(b^2 + b + 2) - (b + 1)^3 = (b - 1)(b^2 + 1),$$

which is positive for $b > 1$. Similarly,

$$J_2(b, 2) + J_3(b, 2) = \log \left( \frac{27(b^2 + b + 4)(b^2 + 2b + 1)}{8(b^2 + 4b + 4)^2} \right),$$

and

$$27(b^2 + b + 4)(b^2 + 2b + 1) - 8(b^2 + 4b + 4)^2 = (b - 1)(19b^3 + 36b^2 + 33b + 20),$$

which is positive for $b > 1$.

Hence $J_2(b, c) + J_3(b, c) > 0$ when $b \geq 2$ and $c = 1$ or $c = 2$. Combining with the results for $J_1(b, c)$, and substituting in equation (13), we conclude that $\frac{d}{db} (RL(b, c) - LL(b, c)) > 0$ for $c = 1$ and $b \geq 4$, and $c = 2$ and $b \geq 3$ as well.

Since the derivative is positive in all cases, it is sufficient to prove that $RL(4, 1) > LL(4, 1)$ and $RL(3, c) > LL(3, c)$. The first one can be verified directly, a computation shows that $RL(4, 1) - LL(4, 1) \approx 0.245$ and thus $RL(4, 1) > LL(4, 1)$. The second inequality, $RL(3, c) > LL(3, c)$, is equivalent to

$$\Delta_c(6) + \Delta_c(5) + \Delta_c(4) + 2\Delta_c(1) > 4\Delta_c(3) + \Delta_c(2).$$

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

$$\int_{c-1}^c \log ((t + 6)(t + 5)(t + 4)(t + 1)^2) \, dt > \int_{c-1}^c \log ((t + 3)^4(t + 2)) \, dt,$$

as $(t + 6)(t + 5)(t + 4)(t + 1)^2 > (t + 3)^4(t + 2)$ for every $t \geq 1$. ♦