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On graph entropy measures based on the number of independent sets and matchings

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In this paper, we consider the graph entropy measures based on the number of independent sets and matchings. The reason to study these measures relates to the fact that the independent set and matching problem is computationally demanding. However, these features can be calculated for smaller networks. In case one can establish efficient estimations, those measures may be also used for larger graphs. So, we establish some upper and lower bounds as well as some information inequalities for these information-theoretic quantities. In order to give further evidence, we also generate numerical results to study these measures such as list the extremal graphs for these entropies. Those results reveal the two entropies possess some new features.

1. Introduction

One of the most fundamental challenges in modern science is to characterize the "complexity" of networked systems [1,2]. Major approaches to measure the complexity are either computable or uncomputable. For example, [3,4]. Graph entropies based on Shannon's entropy formula [5] are classical computable complexity measures. The so-called *structural information content* of a graph was initially introduced in the late 1950s in the context of analyzing biological systems and

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quantifying the information content of the graph [6–8]. This measure is based on symmetry based on the automorphism group of a graph. High complexity means low symmetry and high diversity of the system's elements [9,10], leads to high entropy values, and vice versa.

When comparing graph entropies, other measures of complexity have also been contributed, such as the substructure count [11] and the Kolmogorov complexity [12]. The *substructure count* approach counts the total number of distinct connected subgraphs and uses this quantity as a measure of complexity. It is another computable measure which is based on the idea that the more substructures a system contains, the more complex is the system.

The *Kolmogorov complexity* (K-complexity) has been defined as the minimal length of the program that fully outputs a given string s, when running a universal Turing matching [13,14]. It has been proven to be a more reliable and robust measure compared to Shannon based entropies for graphs as it is independent of graph representations and preselected graph invariants, which are key factors for constructing graph entropy measures [15–17]. The major inconvenience of the K-complexity is that it is lower semi-computable, and there is no effective algorithm to calculate the K-complexity of a given system [18]. However, because it is lower semi-computable, one can find upper bounds on K and short computer programs relative to the length to produce the string [19–21].

Yet, expressing complexity has been intricate because it is in the eye of a beholder. Studying graph entropy measures has been of great importance in various disciplines [10,22,23]. Other properties of graph measures such as uniqueness and structure sensitivity [24,25] could also list. However, an exhaustive study of these properties/weak points on a large variety of graph entropy measures does not yet exist. To the best of our knowledge, Dehmer et al. [26,27] were the first starting with working on these issues when it comes to graph entropies. For more information on this topic, we refer to a survey contributed by Dehmer and Mowshowitz [23].

One of the recently used approach when studying/applying graph entropy measures is based on Dehmer's information functional.

Definition 1 (Dehmer [28])**.** Let G be a graph and $f : S \to \mathbb{R}_+$ be an information functional defined on $S = \{s_1, s_2, \ldots, s_k\}$, where S is a set of elements of G. The entropy of G is defined as

$$\begin{aligned} I_f(G) &= -\sum_{i=1}^{k} \frac{f(s_i)}{\sum_{j=1}^{k} f(s_j)} \log\left(\frac{f(s_i)}{\sum_{j=1}^{k} f(s_j)}\right) \\ &= \log\left(\sum_{i=1}^{k} f(s_i)\right) - \frac{\sum_{i=1}^{k} f(s_i)\log(f(s_i))}{\sum_{j=1}^{k} f(s_j)}, \end{aligned} \tag{1}$$

where "log" denotes the logarithm to the base 2.

Various information functionals have been defined on the basis of metrical properties and other graph invariants, see [23,28–33].

Let G be a simple graph with n vertices and m edges. An *independent set* of G is a set I of vertices of G such that no two vertices in I are adjacent. Denote by $i_k(G)$ the number of independent sets of size k of G. Since the empty set can be thought as an independent set, then $i_0(G) = 1$. The total number of independent sets of G, denoted by $\sigma(G)$, is $\sigma(G) = \sum_{k=0}^{n} i_k(G)$. It has been studied in mathematical chemistry where it is known as the *Merrifield–Simmons index* or *σ-index* [34,35], which is used as a topological index in structural chemistry for quantifying relevant properties of the molecular structure. Define the information functional by $f := i_k(G)$, then we have the following graph entropy.

Definition 2 (Cao et al. [36])**.** Let G be a graph with n vertices. The *entropy based on the number of independent sets* or *NIS entropy* of G, denoted by $I_{nis}(G)$, is defined as

$$I_{nis}(G) = -\sum_{k=0}^{n} \frac{i_k(G)}{\sigma(G)} \log \frac{i_k(G)}{\sigma(G)}. \tag{2}$$

A *matching* of G is a set M of edges in G such that no two edges in M share a common vertex. Denote by $z_k(G)$ the number of matchings of size k of G. Note that the empty set can also be regarded as a matching and thus $z_0(G) = 1$. The total number of matchings of G, denoted by $Z(G)$, is $Z(G) = \sum_{k=0}^{m} z_k(G)$. In the literature [34,35], $Z(G)$ is referred to as *Hosoya index* or *Z-index* and can be used as an index for studying a variety of physico-chemical properties of alkanes. Define the information functional by $f := z_k(G)$, then we have the following graph entropy.

Definition 3 (Cao et al. [36])**.** Let G be a graph with m edges. The *entropy based on the number of matchings* or *NM entropy* of G, denoted by $I_{nm}(G)$, is defined as

$$I_{nm}(G) = -\sum_{k=0}^{m} \frac{z_k(G)}{Z(G)} \log \frac{z_k(G)}{Z(G)}. \tag{3}$$

These two graph entropy measures were introduced by Cao et al. in paper [36] recently. It is worth mentioning that the graph entropy based on the number of matchings was used earlier by Bonchev et al. [37] for testing discrimination of isomers.

In this paper, we further investigate the two graph entropy measures and present the following results.

First, it is a basic problem to calculate entropies for a given graph. However, there are no polynomial algorithms to calculate the NIS and NM entropies for general graphs. The computation is possible for a few graph classes, such as the complete graphs, star graphs, and complete bipartite graphs [36]. We here prove more explicit expressions for the two entropies for sparse and dense graphs.

When we study a graph entropy measure, there are some problems which have attracted the attention of researchers. One of the important problems is: Given a set of graphs $\mathcal{G}$, find upper and lower bounds for the measure or characterize the extremal graphs of the measure. However, this problem has been intricate. Since Shannon's entropy represents a multivariate function and the mass probability distribution are always restricted to some value range when considering graph entropies, we lack appropriate analytical methods to tackle this problem [38]. Bounds and extremal graphs for graph entropies based on degree powers [29,39–44], and distance-based graph entropies [31,33] are presented. Inspired by these results, we state bounds and extremal graphs for the two entropies of connected graphs, trees, and caterpillars with given order. Moreover, we prove the graph which attains the minimal NIS entropy for connected graphs with given order is the complete graph K_n, and the graph which attains the minimal NM entropy for trees with given order is the star S_n. We also propose conjectures for the maximal graphs with respect to the NIS entropy of connected graphs, and extremal graphs with respect to the NM entropy of trees. Extremal graphs which attain the maximal or minimal of the NIS entropy and maximal or minimal of NM entropy for trees or caterpillars with given order are listed based on numerical experiments performed on exhaustively generated graphs.

Another important problem is comparing the NIS and NM entropies with other entropies and topological indices. Gutman et al. established a connection between the Randić index and the graph entropy based on degree power [45]. Inequalities involving information measures for graphs are also referred to as *information inequalities* [46]. For some of the recent contributions in this direction, we refer to [27,46–48] for graph entropies and [49–51] for generalized graph entropies. We also establish information inequalities involving the two graph entropy measures in this paper.

To investigate the NIS and NM entropies in depth, we calculate their values as well as other measures on connected graphs with 5 vertices and perform a comparative study to show that the two entropies exhibit some different features compared to other known measures.

The rest of this paper is organized as follows: We compute these entropies for sparse and dense graphs in Section 2. In Section 3, we present some bounds for the two graph entropy measures with given order and show the extremal graphs with respect to these two entropies. Information inequalities for the two graph entropy measures are presented in Section 4. We compare the two entropies to other measures in Section 5. Summary and conclusion are offered in Section 6.

2. The NIS and NM entropies for sparse and dense graphs

We denote by P_n and C_n the path and cycle on n vertices, respectively. The *independence polynomial* of G is defined as $I(G;x) = \sum_{k=0}^{\alpha(G)} i_k(G)x^k$, where $\alpha(G)$ is the independence number of G. The polynomial is useful for computing the NIS and NM entropies.

Lemma 1 [52]**.** *Some independence polynomials known exactly are the following.*

- $I(P_n, x) = \sum_{k\geq 0} \binom{n+1-k}{k} x^k$.
- $I(C_n, x) = 1 + nx + \sum_{k\geq 2} \frac{n}{k}\binom{n-k-1}{k-1} x^k$.

Let F_n and L_n denote the nth Fibonacci number and Lucas number, respectively. Let $\varphi = (1+\sqrt{5})/2$ and $\phi = (1-\sqrt{5})/5$. Then the Binet form of F_n and L_n are $F_n = (\varphi^n - \phi^n)/\sqrt{5}$ and $L_n = \varphi^n + \phi^n$ for all $n \geq 0$.

Lemma 2 (Prodinger and Tichy [53])**.** *$\sigma(P_n) = F_{n+2}$ and $Z(P_n) = F_{n+1}$ for any $n \geq 0$.*

Lemma 3 (Prodinger and Tichy [53])**.** *$\sigma(C_n) = L_n$ and $Z(C_n) = L_n$ for any $n \geq 3$.*

Proposition 1. *Let P_n be the path with n vertices. Then*

$$I_{nis}(P_n) = \log(F_{n+2}) - \frac{\sum_{k=0}^{\lceil n/2\rceil} \binom{n+1-k}{k} \log\binom{n+1-k}{k}}{F_{n+2}} \tag{4}$$

and

$$I_{nm}(P_n) = \log(F_{n+1}) - \frac{\sum_{k=0}^{\lfloor n/2\rfloor} \binom{n-k}{k} \log\binom{n-k}{k}}{F_{n+1}}, \tag{5}$$

where F_n is the nth Fibonacci number.

Proof. It is easy to see that the independence number of P_n is $\alpha(P_n) = \lceil n/2\rceil$. By Lemma 1, we have $i_k(P_n) = \binom{n+1-k}{k}$ for $0 \leq k \leq \lceil n/2\rceil$. By Lemma 2, $\sigma(P_n) = F_{n+2}$. Therefore, we have

$$I_{nis}(P_n) = \log(F_{n+2}) - \frac{\sum_{k=0}^{\lceil n/2\rceil} \binom{n+1-k}{k} \log\binom{n+1-k}{k}}{F_{n+2}}.$$

It is easy to see that the matching number of P_n is $\alpha'(P_n) = \lfloor n/2 \rfloor$. Note that a matching of size k in P_n corresponds to an independent set of size k in the line graph of P_n, and the line graph of P_n is P_{n-1}. Then, the number of matchings of size k in P_n equals to the number of independent sets of size k in P_{n-1}, i.e., $z_k(P_n) = i_k(P_{n-1}) = \binom{n-k}{k}$. By Lemma 2, $Z(P_n) = F_{n+1}$. Therefore, we have

$$I_{nm}(P_n) = \log(F_{n+1}) - \frac{\sum_{k=0}^{\lfloor n/2 \rfloor} \binom{n-k}{k} \log \binom{n-k}{k}}{F_{n+1}}. \qquad \square$$

Proposition 2. *Let C_n be the cycle with $n \geq 3$ vertices. Then*

$$I_{nis}(C_n) = I_{nm}(C_n) = \log(L_n) - \frac{n \log n + \sum_{k=2}^{\lfloor n/2 \rfloor} \left(\frac{n}{k}\binom{n-k-1}{k-1}\right) \log\left(\frac{n}{k}\binom{n-k-1}{k-1}\right)}{L_n}, \tag{6}$$

where L_n is the nth Lucas number.

Proof. It is easy to see that $\alpha(C_n) = \lfloor n/2 \rfloor$. By Lemma 1, we have $i_k(C_n) = \frac{n}{k}\binom{n-k-1}{k-1}$ for $2 \leq k \leq \lfloor n/2 \rfloor$. Note that $i_0(C_n) = 1$ and $i_1(C_n) = n$. By Lemma 3, $\sigma(C_n) = L_n$. Therefore, we have

$$I_{nis}(C_n) = \log(L_n) - \frac{n \log n + \sum_{k=2}^{\lfloor n/2 \rfloor} \left(\frac{n}{k}\binom{n-k-1}{k-1}\right) \log\left(\frac{n}{k}\binom{n-k-1}{k-1}\right)}{L_n}.$$

Note that a matching of size k in C_n corresponds to an independent set of size k in the line graph of C_n, and the line graph of C_n is C_n. Then, the number of matchings of size k in C_n equals to the number of independent sets of size k in C_n, i.e., $z_k(C_n) = i_k(C_n) = \frac{n}{k}\binom{n-k-1}{k-1}$. Therefore, we have

$$I_{nis}(C_n) = I_{nm}(C_n) = \log(L_n) - \frac{n \log n + \sum_{k=2}^{\lfloor n/2 \rfloor} \left(\frac{n}{k}\binom{n-k-1}{k-1}\right) \log\left(\frac{n}{k}\binom{n-k-1}{k-1}\right)}{L_n}. \qquad \square$$

Let S_n^+ denote the unicyclic graph obtained from the star S_n by adding an edge between two pendent vertices.

Proposition 3. *For the unicyclic graph S_n^+, we have*

$$I_{nis}(S_n^+) = \log(1 + 3 \times 2^{n-3}) - \frac{n \log n + \sum_{k=2}^{n-2} \left(\binom{n-3}{k} + 2\binom{n-3}{k-1}\right) \log\left(\binom{n-3}{k} + 2\binom{n-3}{k-1}\right)}{(1 + 3 \times 2^{n-3})} \tag{7}$$

and

$$I_{nm}(S_n^+) = \log(2n-2) - \frac{n \log n + (n-3)\log(n-3)}{2n-2}. \tag{8}$$

Proof. Suppose that S_n^+ is obtained from S_n by adding an edge between two pendent vertices u and v. Since the number of pendent vertices of S_n^+ is $n-3$, an independent set of size $2 \leq k \leq n-3$ of S_n^+ can be obtained by choosing either k pendent vertices or $k-1$ pendent vertices together with u or v. Thus, we have $i_k(S_n^+) = \binom{n-3}{k} + 2\binom{n-3}{k-1}$. An independent set of size $k = n-2$ can be obtained by choosing $n-3$ pendent vertices together with u or v. Thus, we have $i_{n-2}(S_n^+) = 2$. Note that $i_0(S_n^+) = 1$ and $i_1(S_n^+) = n$. The total number of independent sets of S_n^+ is

$$\begin{aligned}
\sigma(S_n^+) &= 1 + n + \sum_{k=2}^{n-3}\left(\binom{n-3}{k} + 2\binom{n-3}{k-1}\right) + 2 \\
&= 1 + n + 3\sum_{k=1}^{n-3}\binom{n-3}{k} - \binom{n-3}{1} \\
&= 1 + 3 \times 2^{n-3}.
\end{aligned}$$

Therefore

$$I_{nis}(S_n^+) = \log(1 + 3 \times 2^{n-3}) - \frac{n \log n + \sum_{k=2}^{n-2} \left(\binom{n-3}{k} + 2\binom{n-3}{k-1}\right) \log\left(\binom{n-3}{k} + 2\binom{n-3}{k-1}\right)}{(1 + 3 \times 2^{n-3})}.$$

Any pendent edge of S_n^+ together with uv is a matching of size two of S_n^+. Thus, $z_2(S_n^+) = n-3$. Recall that $z_0(S_n^+) = 1$ and $z_1(S_n^+) = n$. Note that $z_k(S_n^+) = 0$ for $k \geq 3$. Hence we have

$$Z(S_n^+) = 1 + n + n - 3 = 2n - 2.$$

Therefore, we have

$$I_{nm}(S_n^+) = \log(2n-2) - \frac{n \log n + (n-3)\log(n-3)}{2n-2}. \qquad \square$$

Proposition 4. *Let G be the graph obtained from K_n by deleting an edge. Then*

$$I_{nis}(G) = \log(n+2) - \frac{n\log n}{n+2} \tag{9}$$

and

$$I_{nm}(G) = \log(Z(G)) - \frac{\left(\binom{n}{2}-1\right)\log\left(\binom{n}{2}-1\right) + \sum_{k=2}^{\lfloor n/2\rfloor}(z_k(G))\log(z_k(G))}{Z(G)}, \tag{10}$$

where $Z(G) = \frac{n(n-1)}{2} + \sum_{k=2}^{\lfloor n/2\rfloor}\frac{(n-2)!}{2^{k-1}(k-1)!(n-2k)!}\left(\frac{n(n-1)}{2k}-1\right)$ *and* $z_k(G) = \frac{(n-2)!}{2^{k-1}(k-1)!(n-2k)!}\left(\frac{n(n-1)}{2k}-1\right)$.

Proof. Since $i_0(G)=1,\ i_1(G)=n,\ i_2(G)=1$ and $i_k(G)=0$ for $3\le k\le n$, we have $\sigma(G)=n+2$. Thus

$$I_{nis}(G) = \log(n+2) - \frac{n\log n}{n+2}.$$

Suppose G is obtained from K_n by deleting an edge uv. It is not hard to get that $z_k(K_n) = \frac{1}{k!}\prod_{j=1}^{k}\binom{n-2j+2}{2}$ for $1\le k\le\lfloor n/2\rfloor$. It follows that the number of matchings of size $k>1$ in K_n containing uv is $\frac{1}{(k-1)!}\prod_{j=1}^{k-1}\binom{n-2j}{2}$. Thus, for $2\le k\le\lfloor n/2\rfloor$, we have

$$\begin{aligned} z_k(G) &= \frac{1}{k!}\prod_{j=1}^{k}\binom{n-2j+2}{2} - \frac{1}{(k-1)!}\prod_{j=1}^{k-1}\binom{n-2j}{2} \\ &= \frac{n!}{2^k k!(n-2k)!} - \frac{(n-2)!}{2^{k-1}(k-1)!(n-2k)!} \\ &= \frac{(n-2)!}{2^{k-1}(k-1)!(n-2k)!}\left(\frac{n(n-1)}{2k}-1\right). \end{aligned}$$

Note that $z_0(G)=1$ and $z_1(G)=\binom{n}{2}-1$. This implies that

$$Z(G) = \frac{n(n-1)}{2} + \sum_{k=2}^{\lfloor n/2\rfloor}\frac{(n-2)!}{2^{k-1}(k-1)!(n-2k)!}\left(\frac{n(n-1)}{2k}-1\right).$$

Therefore, we have

$$I_{nm}(G) = \log(Z(G)) - \frac{\left(\binom{n}{2}-1\right)\log\left(\binom{n}{2}-1\right) + \sum_{k=2}^{\lfloor n/2\rfloor}(z_k(G))\log(z_k(G))}{Z(G)}. \qquad \square$$

3. Bounds and extremal graphs for the NIS and NM entropies of graphs with given order

We first present some lemmas which will be used later.

Lemma 4 (Prodinger et al. [53])**.** *Let G be a tree with n vertices. Then $\sigma(P_n)\le\sigma(G)\le\sigma(S_n)$.*

Throughout this paper, we only consider non-increasing arrangement of each vector in $\mathbb{R}^n$, that is, for any $x=(x_1,\dots,x_n)\in\mathbb{R}^n$, we have $x_1\ge x_2\ge\cdots\ge x_n$.

Definition 4 [54]**.** For $x,y\in\mathbb{R}^n$, $x\prec y$ if

$$\begin{cases} \sum_{i=1}^{k}x_i \le \sum_{i=1}^{k}y_i, & k=1,2,\dots,n-1, \\ \sum_{i=1}^{n}x_i = \sum_{i=1}^{n}y_i. \end{cases} \tag{11}$$

When $x\prec y$, x is said to be *majorized* by y (y *majorizes* x).

Recall that we derive a probability vector p^G from a graph G by either a partition of G or employing an information functional on a certain set of associated objects of G etc. Then the entropy of G is $I(G) = -\sum_{i=1}^{n}p_i\log p_i$, where p_i is the ith entry of p^G and n is the number of entries in p^G. It is clear that $f(x)=-x\log x$ is a concave function when $x>0$. The following lemma can be obtained directly from Theorem 3.1 in [43].

Lemma 5 (Das and Shi [43])**.** *Let H and G be two non-isomorphic graphs of order n such that $p^H\prec p^G$, where p^H and p^G are probability vectors derived from H and G, respectively. Then $I(G)\le I(H)$.*

3.1. Maximal and minimal NIS entropy for graphs with given order

We present the following lower bound for the NIS entropy of connected graphs.

Theorem 1. *Let G be a connected graph on $n \geq 3$ vertices. Then*

$$I_{nis}(K_n) \leq I_{nis}(G). \tag{12}$$

Proof. Let $G_1 \not\cong K_n$ be an arbitrary connected graph on $n \geq 3$ vertices. Consider two probability vectors $p^{G_1} = (p_0^{G_1}, \ldots, p_n^{G_1})$ and $p^{K_n} = (p_0^{K_n}, \ldots, p_n^{K_n})$ derived from the number of independent sets of all sizes of G_1 and K_n, respectively. Without loss of generality, suppose that entries of both p^{G_1} and p^{K_n} are sorted in the non-increasing order.

It is clear that $i_0(K_n) = 1$, $i_1(K_n) = n$ and $i_k(K_n) = 0$ for $k \geq 2$. Thus, $p_0^{K_n} = n/(n+1)$, $p_1^{K_n} = 1/(n+1)$ and $p_k^{K_n} = 0$ for $k \geq 2$. Any non-complete graph has at least one independent set of size at a minimum of two. Hence $i_2(G_1) \geq 1$, $\alpha(G_1) \geq 2$ and $\sigma(G_1) > n+1$, where $\alpha(G_1)$ is the independence number of G_1. Let $i^*(G_1) = \max_k i_k(G_1)$ be the maximum of the number of independent sets of G_1 of all sizes. It follows that $p_0^{G_1} = \frac{i^*(G_1)}{\sigma(G_1)}$. If $i^*(G_1) = n$, then $p_0^{G_1} = n/\sigma(G_1) < n/(n+1) = p_0^{K_n}$. Since $i_2(G_1) \geq 1$, it is implied that $p_0^{G_1} + p_1^{G_1} < 1$. Note that $p_0^{K_n} + p_1^{K_n} = 1$, implying that $p_0^{K_n} + p_1^{K_n} > p_0^{G_1} + p_1^{G_1}$. Thus, we have $p^{K_n} \succ p^{G_1}$. By Lemma 5, $I_{nis}(K_n) \leq I_{nis}(G_1)$. If $i^*(G_1) > n$, then the size r, of which the number of independent sets attains $i^*(G_1)$, is greater than or equal to 2. Since $i_n(G_1) > 0$ if, and only if, G_1 is the empty graph we may assume that $r < n$. Consider an associated bipartite graph $G_2 = [X, Y]$ in which X represents the set of independent sets of size $r > 1$ of G_1, Y the set of independent sets of size $r-1$ of G_1, and an edge xy with $x \in X$ and $y \in Y$ if and only if the independent set I_r represented by x and the independent set I_{r-1} represented by y satisfying $I_{r-1} \subset I_r$. An independent set I_r of size r contains respective r independent sets of size $r-1$, each of which is a subset of I_r, implying that for each $x \in X$ there are r edges incident to x. That is, the number of edges of G_2 is $i_r(G_1) \cdot r$. On the other hand, for an independent set I_{r-1} of size $r-1$, the number of vertices in $V(G_1) \backslash I_{r-1}$ which are not adjacent to I_{r-1} is at most $n-r$ (recall that G_1 is connected). Hence, there are at most $n-r$ independent sets of size r containing I_{r-1}. Thus, for each vertex $y \in Y$, the number of edges incident to y is at most $n-r$. Consider the number of edges $e(G_2)$ of G_2, we have

$$i_r(G_1) \cdot r = e(G_2) \leq i_{r-1}(G_1) \cdot (n-r).$$

That is,

$$i_{r-1}(G_1) \geq \frac{r}{n-r} \cdot i_r(G_1).$$

Thus, we have

$$p_0^{G_1} = \frac{i_r(G_1)}{\sigma(G_1)} \leq \frac{i_r(G_1)}{i_r(G_1) + i_{r-1}(G_1)} \leq \frac{i_r(G_1)}{i_r(G_1) + \frac{r}{n-r} i_r(G_1)} < \frac{n}{n+1}. \tag{13}$$

That is, $p_0^{G_1} < p_0^{K_n}$. Recall that $p_0^{K_n} + p_1^{K_n} = 1 > p_0^{G_1} + p_1^{G_1}$. Hence, $p^{K_n} \succ p^{G_1}$. By Lemma 5, $I_{nis}(K_n) \leq I_{nis}(G_1)$. Therefore, $I_{nis}(K_n) \leq I_{nis}(G)$. □

To study extremal connected graphs with respect to the NIS entropy further, we did numerical experiments and searched graphs with maximal NIS entropy. Based on results of numerical experiments performed on exhaustively generated graphs, we propose the following conjecture.

Conjecture 1. *Let G be a connected graph on $n \geq 4$ vertices. Then*

$$I_{nis}(G) \leq I_{nis}(S_n). \tag{14}$$

Moreover, we also performed numerical experiments on exhaustively generated trees with at most 18 vertices. Let T be a tree on n vertices. The maximum of $I_{nis}(T)$ is attained when T is the star graph S_n. The minimum of $I_{nis}(T)$ is attained when T is the path graph P_n except the case $n = 7$. If $n = 7$, then the minimum of $I_{nis}(T)$ is attained when T is the graph $G284$ (p.69 of Read and Wilson [55], see Fig. 1.) rather than P_7.

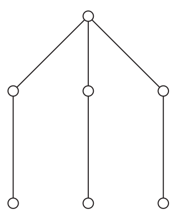


Fig. 1. The graph $G284$.

At last, we did numerical experiments on exhaustively generated caterpillars. A *caterpillar* is a tree such that its internal vertices induce a path. Caterpillar graphs are special trees which have been used in chemistry to study combinatorial and physical properties of benzenoid hydrocarbons [56]. By numerical experiments, we obtained that for caterpillars of order n, the path graph P_n minimizes the NIS entropy, whereas the star graph S_n maximizes it.

3.2. Maximal and minimal NM entropy for graphs with given order

First, we list the extremal graphs with respect to the NM entropy for further study.

A *generalized star* S^* is a tree consisting of several paths, called *branches*, with the unique common endvertex.

By calculating NM entropy for exhaustively generated graphs within 9 vertices, we find that the star graph S_n always attains the minimal NM entropy of connected graphs with n vertices. However, the cases that graphs attain the maximal NM entropy are a little complicated. The graphs with maximal values of NM entropy with 6, 7, 8 and 9 vertices are shown in Fig. 2. Based on these results, we present the following conjecture.

Conjecture 2. *Let G be a graph on $n > 5$ vertices. Then*

$$I_{nm}(S_n) \le I_{nm}(G) \le I_{nm}(S_n^*), \tag{15}$$

where S_n^* is the generalized star with branches whose lengths differ at most 1.

It is interesting that the extremal connected graphs (maximal and minimal) with respect to the NM entropy are trees. We present the following lower bound for the NM entropy of trees. The left-hand side of Inequality (15) has been proven for trees (see Theorem 2).

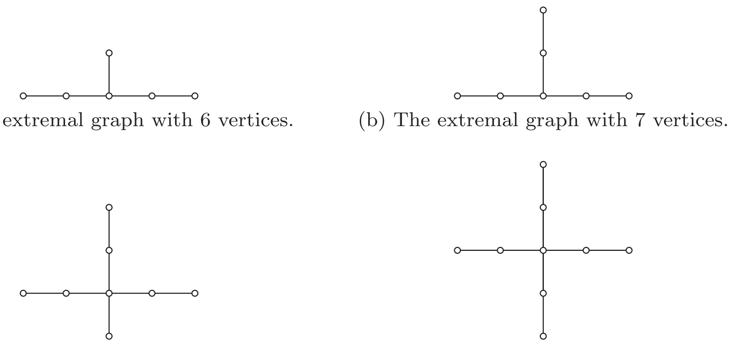
Theorem 2. *Let T be a tree on $n > 3$ vertices. Then*

$$I_{nm}(S_n) \le I_{nis}(T). \tag{16}$$

Proof. Let $T_1 \ncong S_n$ be an arbitrary tree on $n > 3$ vertices. Consider two probability vectors $p^{T_1} = (p_0^{T_1}, \ldots, p_n^{T_1})$ and $p^{S_n} = (p_0^{S_n}, \ldots, p_n^{S_n})$ derived from the number of matchings of all sizes of T_1 and S_n, respectively. Without loss of generality, suppose that entries of both p^{T_1} and p^{S_n} are sorted in the non-increasing order.

It is clear that $z_0(S_n) = 1,\ z_1(S_n) = n - 1$ and $z_k(S_n) = 0$ for $k \ge 2$. Thus, $p_0^{S_n} = (n-1)/n,\ p_1^{S_n} = 1/n$ and $p_k^{S_n} = 0$ for $k \ge 2$. Any tree which is not a star has at least one matching of size at a minimum of two. Hence $z_2(T_1) \ge 1$, $\alpha'(T_1) \ge 2$ and $Z(T_1) > n$, where $\alpha'(T_1)$ is the matching number of T_1. Let $z^*(T_1) = \max_k z_k(T_1)$ be the maximum of the number of matchings of T_1 of all sizes. It follows that $p_0^{T_1} = \frac{z^*(T_1)}{Z(T_1)}$. If $z^*(T_1) = n - 1$, then $p_0^{T_1} = (n-1)/Z(T_1) < n - 1/n = p_0^{S_n}$. Since $z_2(T_1) \ge 1$, it is implied that $p_0^{T_1} + p_1^{T_1} < 1$. Note that $p_0^{S_n} + p_1^{S_n} = 1$, implying that $p_0^{S_n} + p_1^{S_n} > p_0^{T_1} + p_1^{T_1}$. Thus, we have $p^{S_n} \succ p^{T_1}$. By Lemma 5, $I_{nm}(S_n) \le I_{nm}(T_1)$. If $z^*(T_1) > n - 1$, then the size r, of which the number of matchings attains $z^*(T_1)$, is greater than or equal to 2. Note that $\alpha'(T) \le \lceil \frac{n}{2} \rceil$ for any tree. Hence $r < n$. Consider an associated bipartite graph $G_2 = [X, Y]$ in which X represents the set of matchings of size $r > 1$ of T_1, Y the set of matchings of size $r - 1$ of T_1, and an edge xy with $x \in X$ and $y \in Y$ signifies that $y \subset x$ if and only if the matching M_r represented by x and the matching M_{r-1} represented by y satisfying $M_{r-1} \subset M_r$. A matching M_r of size r contains respective r matchings of size $r - 1$, each of which is a subset of M_r, implying that for each $x \in X$ there are r edges incident to x. That is, the number of edges of G_2 is $z_r(T_1) \cdot r$. On the other hand, for a matching M_{r-1} of size $r - 1$, the number of edges in $e(T_1) \backslash M_{r-1}$ is at most $n - r - 1$, where $e(T_1)$ is the number of edges of T_1. Hence, there are at most $n - r - 1$ matchings of size r containing M_{r-1}. Thus, for each vertex $y \in Y$, the number of edges incident to y is at most $n - r - 1$. Consider the number of edges $e(G_2)$ of G_2, we have

$$z_r(T_1) \cdot r = e(G_2) \le z_{r-1}(T_1) \cdot (n - r - 1).$$



(a) The extremal graph with 6 vertices. (b) The extremal graph with 7 vertices.

(c) The extremal graph with 8 vertices. (d) The extremal graph with 9 vertices.

Fig. 2. Graphs attain the maximal NM entropy with given order.

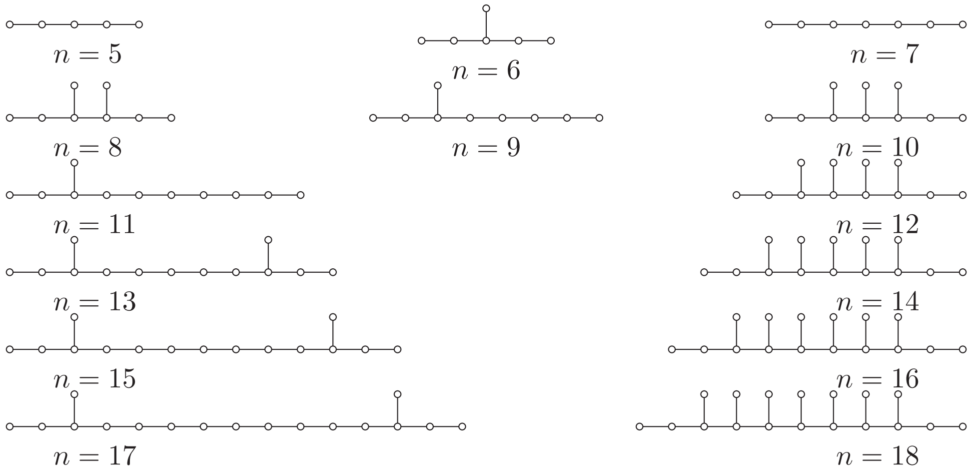


Fig. 3. Caterpillars with maximal NM entropy with given order.

That is,

$$z_{r-1}(T_1) \geq \frac{r}{n-r-1} \cdot z_r(T_1).$$

Thus, we have

$$p_0^{T_1} = \frac{z_r(T_1)}{Z(T_1)} \leq \frac{z_r(T_1)}{z_r(T_1) + z_{r-1}(T_1)} \leq \frac{z_r(T_1)}{z_r(T_1) + \frac{r}{n-r-1} z_r(T_1)} < \frac{n-1}{n}. \tag{17}$$

That is, $p_0^{T_1} < p_0^{S_n}$. Recall that $p_0^{S_n} + p_1^{S_n} = 1 > p_0^{T_1} + p_1^{T_1}$. Hence, $p^{S_n} \succ p^{T_1}$. By Lemma 5, $I_{nm}(S_n) \leq I_{nm}(T_1)$. Therefore, $I_{nm}(S_n) \leq I_{nm}(T)$. □

We also searched the caterpillars with extremal NM entropy with, at most, 18 vertices. Obviously, among all caterpillars of order n, the minimal NM entropy is attained by the star S_n. The result for the maximal NM entropy appears to be less intuitive. Caterpillars with respect to maximal NM entropy with n $(5 \leq n \leq 18)$ vertices are presented in Fig. 3. It is noticed that, for caterpillars with sufficiently large order n $(n \geq 12)$, the structures of extremal graphs which attain the maximal NM entropy are similar and decided by parity of their orders.

4. Information inequalities for the NIS and NM entropies

Lemma 6 (Galvin [57]). *Fix n and k with $n > 4$ and $3 \leq k \leq n-1$. If G is an n-vertex graph with minimum degree at least 1 and $G \ncong K_{1,n-1}$, then $i_k(G) < i_k(K_{1,n-1})$.*

Lemma 7 (Maximum of the uniform). *Let G be a graph and $f : S \to \mathbb{R}_+$ be an information functional defined on a certain set $S = \{s_1, s_2, \ldots, s_k\}$ of associated objects of G. Then*

$$I_f(G) \leq \log k,$$

with equality if, and only if, $f(s_1) = f(s_2) = \cdots = f(s_k)$.

Lemma 8 (Chen et al. [40]). *Let p_i and p_i^* be the probabilities of two probability vectors p and p^* with lengths n, respectively. If $p_i\alpha \leq p_i^*$ for each i and $\alpha < 1$ is a constant, then*

$$I(p) > \log(\alpha) - \sum_{i=1}^{n} p_i \log(p_i^*). \tag{18}$$

Proposition 5. *Let G be a graph with independence number $\alpha(G)$. Then, we have*

$$I_{nis}(G) \leq \log(\alpha(G) + 1). \tag{19}$$

Proof. It is clear that $i_k(G) = 0$ for $\alpha(G) < k \leq n$, where n is the number of vertices of G. Then

$$I_{nis}(G) = -\sum_{k=0}^{n} \frac{i_k(G)}{\sigma(G)} \log\left(\frac{i_k(G)}{\sigma(G)}\right) = -\sum_{k=0}^{\alpha(G)} \frac{i_k(G)}{\sigma(G)} \log\left(\frac{i_k(G)}{\sigma(G)}\right).$$

By Lemma 7, $I_{nis}(G) \leq \log(\alpha(G)+1)$ with equality if and only if $i_0(G) = i_1(G) = \cdots = i_{\alpha(G)} = 1$. □

Based on Lemma 6, we derive the following result straightforwardly.

Proposition 6. *Let G be a graph with n vertices and minimum degree at least 1. Then we have*

$$\log(\sigma(G)) - \frac{n\log n + (\alpha(G)-1)\left(\binom{n-1}{\lfloor\frac{n-1}{2}\rfloor}+1\right)\log\left(\binom{n-1}{\lfloor\frac{n-1}{2}\rfloor}+1\right)}{\sigma(G)} \le I_{nis}(G) \le \log(\sigma(G)) - \frac{n\log n}{\sigma(G)}, \tag{20}$$

where $\alpha(G)$ is the independence number of G and $\sigma(G)$ is the σ-index of G.

Proof. Recall that $i_0(G)=1,\ i_1(G)=n$ and $i_k(G)=0$ for $k>\alpha(G)$. By Eq. (1), we have

$$I_{nis}(G) = \log(\sigma(G)) - \frac{\sum_{k=0}^{n} i_k(G)\log(i_k(G))}{\sigma(G)} = \log(\sigma(G)) - \frac{n\log n + \sum_{k=2}^{\alpha(G)} i_k(G)\log(i_k(G))}{\sigma(G)}.$$

Let $g(x)=x\log x$. Note that $g'(x)=\log x+\frac{1}{\ln 2}$, implying $g'(x)>0$ for $x\ge 1$. By the monotonicity property of $g(x)$, we yield $0\le \sum_{k=2}^{\alpha(G)} i_k(G)\log(i_k(G)) \le (\alpha(G)-1)i^*(G)\log(i^*(G))$, where $i^*(G)=\max_k i_k(G)$ is the maximum of the number of independent sets of G of all sizes. (Recall that $i_k(G)\ge 1$ for $2\le k\le \alpha(G)$.) By Lemma 6, we have $i^*(G)\le i^*(K_{1,n-1})=\binom{n-1}{\lfloor\frac{n-1}{2}\rfloor}+1$. Thus, $0\le \sum_{k=2}^{\alpha(G)} i_k(G)\log(i_k(G)) \le (\alpha(G)-1)\left(\binom{n-1}{\lfloor\frac{n-1}{2}\rfloor}+1\right)\log\left(\binom{n-1}{\lfloor\frac{n-1}{2}\rfloor}+1\right)$. Therefore,

$$\log(\sigma(G)) - \frac{n\log n+(\alpha(G)-1)\left(\binom{n-1}{\lfloor\frac{n-1}{2}\rfloor}+1\right)\log\left(\binom{n-1}{\lfloor\frac{n-1}{2}\rfloor}+1\right)}{\sigma(G)} \le I_{nis}(G) \le \log(\sigma(G)) - \frac{n\log n}{\sigma(G)}.$$

This is the desired inequality (20). □

Proposition 7. *Let $G\not\cong S_n$ be a connected graph on n vertices. Then*

$$I_{nis}(G) \ge \log\left(\frac{\sigma(G)}{\sigma(S_n)}\right) - \sum_{k=0}^{n} p(i_k(G))\log(p(i_k(S_n))). \tag{21}$$

Proof. Recall that $i_k(G)\le i_k(S_n)$ for $0\le k\le n$. Hence $\sigma(G)<\sigma(S_n)$. Thus we have

$$p(i_k(G)) = \frac{i_k(G)}{\sigma(G)} < \frac{i_k(S_n)}{\sigma(G)} = \frac{i_k(S_n)}{\sigma(S_n)}\cdot\frac{\sigma(S_n)}{\sigma(G)} = \frac{\sigma(S_n)}{\sigma(G)}p(i_k(S_n)).$$

That is,

$$p(i_k(G))\frac{\sigma(G)}{\sigma(S_n)} < p(i_k(S_n)).$$

Recall that $\sigma(G)<\sigma(S_n)$. Thus by Lemma 8, we have

$$I_{nis}(G) \ge \log\left(\frac{\sigma(G)}{\sigma(S_n)}\right) - \sum_{k=0}^{n} p(i_k(G))\log(p(i_k(S_n))).$$ □

From the result of Lemma 7, we can also infer

Proposition 8. *Let G be a graph with matching number $\alpha'(G)$. Then we have*

$$I_{nm}(G) \le \log(\alpha'(G)+1). \tag{22}$$

Proof. It is clear that $z_k(G)=0$ for $\alpha'(G)<k\le m$, where m is the number of edges of G. Then

$$I_{nm}(G) = -\sum_{k=0}^{m}\frac{z_k(G)}{Z(G)}\log\frac{z_k(G)}{Z(G)} = -\sum_{k=0}^{\alpha'(G)}\frac{z_k(G)}{Z(G)}\log\frac{z_k(G)}{Z(G)}.$$

By Lemma 7, $I_{nm}(G)\le\log(\alpha'(G)+1)$ with equality if and only if $z_0(G)=z_1(G)=\cdots=z_{\alpha'(G)}=1$. □

Similar to the NIS entropy, we have

Proposition 9. *Let G be a graph with m edges. Then we have*

$$\log(Z(G)) - \frac{m\log m + (\alpha'(G)-1)z^*(G)\log(z^*(G))}{Z(G)} \le I_{nm}(G) \le \log(Z(G)) - \frac{m\log m}{Z(G)}, \tag{23}$$

where $\alpha'(G)$ is the matching number of G, $Z(G)$ is the Z-index of G and $z^*(G) = \max\limits_k z_k(G)$ is the maximum of the number of matchings of G of all sizes.

Proof. It is trivial that $z_0(G) = 1,\ z_1(G) = m$ and $z_k(G) = 0$ for $k > \alpha'(G)$. By applying Eq. (1), we conclude

$$I_{nm}(G) = \log(Z(G)) - \frac{\sum_{k=0}^{m} z_k(G)\log(z_k(G))}{Z(G)}$$
$$= \log(Z(G)) - \frac{m\log m + \sum_{k=2}^{\alpha'(G)} z_k(G)\log(z_k(G))}{Z(G)}.$$

Let $g(x) = x\log x$. Note that $g'(x) = \log x + \frac{1}{\ln 2}$, implying $g'(x) > 0$ for $x > 1$. By the monotonicity property of $g(x)$, we yield $0 \le \sum_{k=2}^{\alpha'(G)} z_k(G)\log(z_k(G)) \le (\alpha'(G)-1)z^*(G)\log(z^*(G))$. Thus,

$$\log(Z(G)) - \frac{m\log m + (\alpha'(G)-1)z^*(G)\log(z^*(G))}{Z(G)} \le I_{nm}(G) \le \log(Z(G)) - \frac{m\log m}{Z(G)}. \qquad \square$$

Proposition 10. *Let $G \not\cong K_n$ be a connected graph on n vertices and m edges. Then*

$$I_{nm}(G) \ge \log\left(\frac{Z(G)}{Z(K_n)}\right) - \sum_{k=0}^{m} p(z_k(G))\log(p(z_k(K_n))). \tag{24}$$

Proof. Recall that $z_k(G) \le z_k(K_n)$ for $0 \le k \le n$. Hence $Z(G) < Z(K_n)$. Thus we have

$$p(z_k(G)) = \frac{z_k(G)}{Z(G)} < \frac{z_k(K_n)}{Z(G)} = \frac{z_k(K_n)}{Z(K_n)} \cdot \frac{Z(K_n)}{Z(G)} = \frac{Z(K_n)}{Z(G)}p(z_k(K_n)).$$

That is,

$$p(z_k(G))\frac{Z(G)}{Z(K_n)} < p(z_k(K_n)).$$

Recall that $z(G) < z(K_n)$. Thus by lemma 8, we have

$$I_{nm}(G) \ge \log\left(\frac{Z(G)}{Z(K_n)}\right) - \sum_{k=0}^{m} p(z_k(G))\log(p(z_k(K_n))). \qquad \square$$

5. Comparison of NIS and NM entropies to other measures

The graphs for numerical experiments are presented in Fig. 4 arranged increasingly according to their topological complexity *TC*, which is defined as the sum of the total adjacencies of all subgraphs [15]. It is a non-entropy-based approach that uses the subgraph count idea to measuring complexity and is considered more stable.

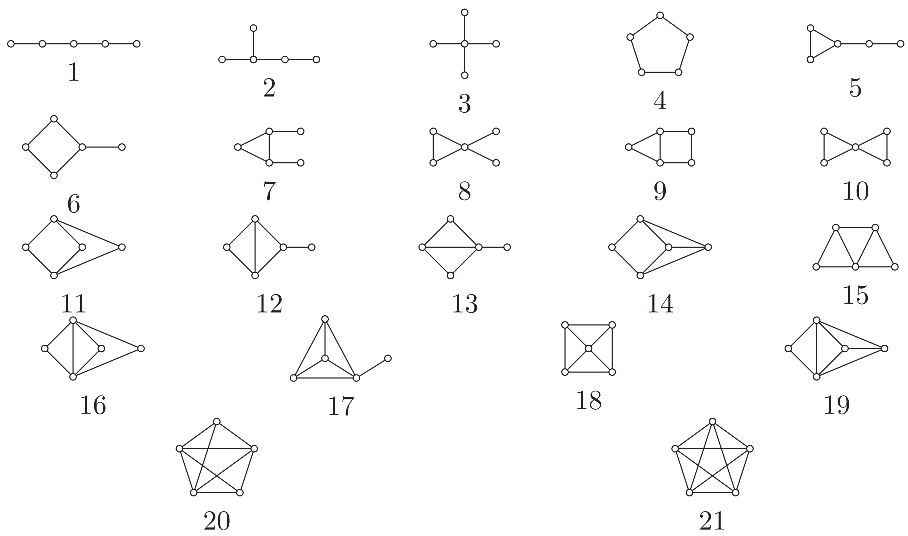


Fig. 4. All simple connected graphs with 5 vertices sorted according their topological complexity *TC*.

The classical *topological information content* I_α due to Mowshowitz [8] is based on using the vertex orbits $n_1, n_2, \ldots, n_k$. I_α is given by the formula

$$I_\alpha = -\sum_{i=1}^{k} p_i \log p_i = -\sum_{i=1}^{k} \frac{n_i}{n} \log \frac{n_i}{n}. \tag{25}$$

Bonchev [58] defined a measure I_{vd} for a graph G calculated by

$$I_{vd} = -\sum_{i=1}^{n} d_i \log d_i, \tag{26}$$

where d_i is the degree of vertex v_i of G. It is regarded as a more adequate complexity measure.

The *entropy based on degree power* is one of the most popular entropy measure [29]. It has been defined by

$$I_d^k = -\sum_{i=1}^{n} \frac{d_i^k}{\sum_{j=1}^{n} d_j^k} \log \frac{d_i^k}{\sum_{j=1}^{n} d_j^k}. \tag{27}$$

In this paper we set the parameter $k = 1$ and use I_d as an entropy measures.

The values of these measures are calculated and presented in Table 1. The graphs are separated by lines according to different number of cycles. The values of I_α presented in the table show that graphs 4 and 21 attain the same minimum entropy. This is because vertices in both two graphs have one orbit only and, thus, the entropy equals 0. The result indicates that they have the same complexity from the point view of I_α. It is observed that both graphs 4 and 21 also have the same value of I_d, since they are regular graphs, and I_d is only related to the order ($I_d(G) = \log n$ for any non-empty regular graph G with n vertices). From the K-complexity point of view, both the two regular graphs 4 and 21 are easy to describe. Thus, they should have low K values. Yet, one should also pay attention that not all regular graphs are easy to describe, for example, the Petersen graph. The measure I_d produces very high values for regular graphs despite some of them exhibit low complexity. Notice that the graphs 2, 5, 6, 11, 12 have high I_α values, since the number of orbits of vertices in these graphs are more than one, and vertices in different orbits nearly uniformly distributed. From the K-complexity point of view, these graphs are non-regular and not easy to describe. Thus, they have high K values. But we also notice that the graph 16 has a much lower value of I_α than the graph 1 while the graph 1 is much easier to describe.

The graph 21 has higher value of *TC* than the graph 4. This is due to the subgraph count approach counts each subgraph, and the graph 21 has more substructures. Experiments show that the graph 4 has a lower I_{vd} while the graph 21 has a higher one. It holds because the degree of each vertex in graph 21 is higher than the quantity in 4. There exist more connections in the graph 21 and, thus, a higher complexity in point view of connection. In fact, the measure I_{vd} is considered to be more meaningful than I_α as it satisfies the criteria of nice complexity measure better, such as increases with the connectivity and other complexity factors (e.g., number of branches, cycles, cliques), see [58]. By using K-complexity, we see that a large number of substructures does not always mean high complexity. This implies that *TC* and I_{vd} are suitable complexity measures but only by taking specific aspects of complexity into account. Moreover, the measure *TC* weights each subgraph using connections in it and adds up weights as the measure of complexity, and the measure I_{vd} uses connections

Table 1
The Shannon's entropies and *TC* of connected graphs with 5 vertices.

Graphs	I_α	I_d	I_{nis}	I_{nm}	I_{vd}	*TC*
1	1.522	2.25	1.643	1.406	6	60
2	1.922	2.156	1.727	1.379	6.755	76
3	0.722	2	2.022	0.722	8	100
4	0	2.322	1.349	1.349	10	160
5	1.922	2.242	1.349	1.361	10.755	172
6	1.922	2.246	1.650	1.361	10.755	290
7	1.522	2.171	1.650	1.352	11.51	212
8	1.522	2.122	1.760	1.299	12	230
9	1.522	2.292	1.361	1.314	15.51	482
10	0.722	2.252	1.361	1.325	16	292
11	0.971	2.292	1.677	1.314	15.51	504
12	1.922	2.292	1.361	1.314	16.265	511
13	1.922	2.189	1.677	1.322	16.755	566
14	1.522	2.306	1.352	1.272	21.02	1278
15	1.522	2.271	1.352	1.287	21.51	1316
16	0.971	2.236	1.685	1.296	22	1394
17	1.371	2.217	1.352	1.296	22.265	1396
18	0.722	2.311	1.298	1.236	27.02	3216
19	1.522	2.281	1.299	1.252	27.51	3290
20	0.971	2.308	1.149	1.207	33.51	7806
21	0	2.322	0.650	1.169	40	18,180

(degrees) between vertices to construct entropy based complexity. Thus, TC is focusing on the number of substructures and connections between different substructures while I_{vd} is focusing on connections between substructures. So we get an increasing order $1 \to 2 \to 3$ for the first three graphs according to their TC values. The same holds for the measure I_{vd}. It is obvious that the graph 3 is easier to describe than the graph 2. Thus, the graph 3 should have a lower K value than the graph 2. It seems that the connection is a certain aspect of complexity that the K-complexity sometimes neglect. We also notice that the graphs 5 and 6 have the same I_{vd} value where the graph 6 has a longer cycle length than graph 5. Notice that the cycle length is another aspect of complexity in some sense. If the cycle length is taken into account, the measure TC gets a higher value for the graph 6 than the graph 5 while I_{vd} relatives to the degree sequence in such a way it neglects the cycle length and, hence, obtains the same value for graphs 5 and 6.

It is observed that the graph 21 attains the minimum of I_{nis} and the graph 4 attains the maximum of I_{nis} while the graph 21 attains the maximum of I_{nm} and the graph 4 attains the minimum of I_{nm} among these graphs. The contradicting results reveal that both I_{nis} and I_{nm} may overestimate complexity for some graphs. Given the fact that the Shannon entropy is an information measure and it has been used to quantify uncertainty, we see that the I_{nis} entropy might be suitable for measuring uncertainty of vertex independence. That is, if the number of independent sets of different sizes are equally like, then I_{nis} exhibits a relative high value, as it is most difficult to predict the outcome from the set of all independent sets. If the number of independent sets of different sizes are not fair, then there is less uncertainty, and some independent sets of some particular size are more likely occur. Moreover, since the number of independent sets of size 0 and 1 in any non-empty graph of order n are 1 and n, respectively, a graph with high I_{nis} value always has more independent sets of size greater than one. If we randomly chose a vertex subset V_s from a graph with high I_{nis}, the probability that V_s to be an independent set is high. For example, the graph 8 has a higher I_{nis} value than the graph 7, because the graph 8 has two independent sets of size 3 while graph 7 has only one. That is, if we randomly chose 3 vertices in the two graphs respectively, there is a higher probability that the 3 vertices chosen from the graph 8 to be an independent set than the vertices chosen from the graph 7 be an independent set. One should also notice that the results of using I_{nis} to compare uncertainty of vertex independence may be only correct for graphs with the same number of vertices and edges. For two graphs with the same number of vertices but different number of edges, the situation is that complicated and may not be useful. The NM entropy behaves equally but for measuring the uncertainty of edge independence.

The graphs 4 and 21 have a relatively high vertex and edge independence, respectively. This results in higher I_{nis} and I_{nm} for the two graphs, respectively. It is very interest that the graphs 5 and 6 have the same value of I_{nm}. Notice that these two graphs also have the same values of I_{α} and I_{vd}. This implies that the two graphs have the same complexity in some sense (uncertainty of edge independence). But the two graphs have different values of I_{nis} while the graphs 6 and 7 have the same value of I_{nis}, implying the two graphs have the same uncertainty when considering vertex independence.

One may note that low entropy values always imply low K-complexity for graphs.

The inspection of Table 1 reveals that most measures, except TC, are strongly degenerate and cannot discriminate well between structures. Mathematical chemists always hope to pursue a nice measure which could discriminate each graphs uniquely. This means non-isomorphic graphs should have different values. Consider that two non-isomorphic graphs may have exactly the same complexity, it is very challenging to establish a nice complexity measure that could get exactly the same value for these non-isomorphic graphs having the same complexity.

6. Summary

In this paper, we have studied graph entropy measures based on the number of independent sets and matchings. We present some explicit expressions for the NIS and NM entropies for sparse and dense graphs. We also prove the graph which attains the minimal NIS entropy for connected graphs with given order is the complete graph K_n and the graph which attains the minimal NM entropy for trees with given order is the star S_n. Moreover, we propose conjectures for the maximal graphs with respect to the NIS entropy of connected graphs and extremal graphs with respect to the NM entropy of trees based on numerical experiments. We also list extremal graphs which attain the maximal or minimal of the NIS entropy and maximal or minimal of NM entropy for trees or caterpillars with given order for further search.

In addition to investigating these two entropies with other known measures, we present some information inequalities involving the NIS entropy with Independence number or σ-index, and the NM entropy with matching number or Z-index, respectively. Those results will trigger further investigations when proving further properties.

We also performed a comparison of the NIS and NM entropies with the subgraph count approach based measure TC, entropies I_{α}, I_d and I_{vd}, and the K-complexity. Our results revealed that the NIS and the NM entropy are not suitable complexity measures in view of an important definition due to Bonchev [59]. In fact, Bonchev [59] described what kind of features should a meaningful complexity measure possess. We saw that graph entropies always need preselected graph invariants which are very specific and cannot characterize the overall topology of a network. Moreover, entropies often capture symmetry of a graph. The notion of complexity is an intricate and versatile concept while symmetry could have a simplifying meaning [60].

There are still further interesting open questions for future work. For instance, it would be valuable to find extremal graphs for the NIS and NM entropies for various classes of graphs and to rank graphs with respect to these entropies for further analyses. Comparing different graph entropies remains an open problem. It is of great significance to compare and analyze different entropies as one could approximate entropies which are demanding to calculate by ones which are computationally more approachable, assuming that they capture structural information similarly. Analytical methods to compare graph entropies with more graph topological indices, e.g., inequalities would be also worthwhile to establish in the future.

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