# Connections between generalized graph entropies and graph energy 

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#### Abstract

Dehmer and Mowshowitz introduced a class of generalized graph entropies by using known information-theoretic measures. These measures rely on assigning a probability distribution to a graph. In this article, we prove some extremal properties of such generalized graph entropies by employing the graph energy and the spectral moments. Moreover, we study the relationships between the generalized graph entropies and compute the values of the generalized graph entropies for special graph classes.


Key words: information theory; entropy; graph entropy; graph energy; graph spectrum

## 1 Introduction

The entropy of a graph is an information-theoretic quantity that has been introduced by Mowshowitz [33]. This quantity expressing the complexity of a graph is based on the well-known Shannon entropy [8, 40]. Importantly, Mowshowitz interpreted his graph entropy measure as the structural information content (of a graph) and proved several important properties thereof, see, e.g., [33, 34, 35, 36]. Later, Körner developed a different measure also
called graph entropy in the context of information theory [29]. An up-to-date review on graph entropy measures has recently been published by Dehmer and Mowshowitz [14]. Historically, the research on the information content of graphs started in the fifties when investigating chemical and biological systems $[32,37,41]$. A central problem in this area relates to determine the structural complexity of chemical and biological systems representing complex networks. For instance, various information-theoretic measures (and also non-information-theoretic measures) and other techniques have been developed to determine the structural complexity of molecular structures and complex networks $[4,3,11,17,15,18]$. But those studies revealed that there is no unique measure/method to determine the structural complexity of graphs as it depends on various factors such as the number of edges, vertices, paths, cycles etc. As a result, Bonchev and his co-workers outlined some concepts of topological complexity and stated rules that such a meaningful concept should fulfill [5]. In [25, 39], the authors introduced the concept of "set-complexity", based on a context-dependent measure of information, and used this concept to describe the complexity of gene interaction networks. The binary graphs and edge-colored graphs are studied and the relation between complexity and structure of these graphs is examined in detail. In contrast, we put the emphasis on analyzing properties of spectra-based entropies and study interrelations thereof.

We emphasize that various graph entropy measures have been developed $[4,14,33]$. For example, partitions by using several graph invariants such as vertices, edges, distances and so forth have been used to assign a probability distribution to a graph. Prominent examples thereof are the magnitude-based information indices due to Bonchev [4] and the topological information content developed by Rashewsky [37]. For the latter measure, see also the seminal work of Mowshowitz [33]. Another class of graph entropy measures has been developed by Dehmer [11]. Here a probability value is assigned to each indiviual vertex by using so-called information functionals [11] (see Section 3). Recently, Dehmer et al. also developed a graph entropy measure by using the moduli of the eigenvalues of a graph by employing several graph theoretical matrices [16]. They proved that this measure (among others) has high discrimination power by using chemical structures and exhaustively generated graphs. Also, so-called generalized graph entropies have been investigated due to Dehmer and Mowshowitz by applying generalized entropy measures, see [13].

In this paper, we use the mentioned generalized graph entropy measures and express those quantity by using the energy and spectral moments of graphs [20]. The paper is organized as follows: in Section 2, we introduce the definition and some elementary results on spectra of graphs and graph energy. In Section 3, we state the definitions of the generalized graph entropies, which was introduced by Dehmer and Mowshowitz in [13]. In Section 4, we prove some extremal properties of such generalized graph en-
tropies by employing the graph energy and the spectral moments. Moreover, we give some inequalities between the generalized graph entropies. In Section 5, we compute the values of the generalized graph entropies for special graph classes. The paper finishes in Section 6 with a summary and conclusion.

## 2 Spectra of graphs and graph energy

Let $G=(V, E)$ be a graph with $n$ vertices and $m$ edges. Let $A(G)$ be the adjacency matrix of $G$. The eigenvalues $\lambda_{1}, \lambda_{2}, \ldots, \lambda_{n}$ of the the matrix $A(G)$ are said to be the eigenvalues of graph $G$ and to form its spectrum. The $k$-th spectral moment of graph $G$ is defined as $M_{k}(G)=\sum_{i=1}^{n} \lambda_{i}^{k}$. Observe that for odd $k, M_{k}(G)=0$ if $G$ is a bipartite graph. In order to overcome this limitation, the authors in [43] defined the moment-like quantities, $M_{k}^{*}(G)=$ $\sum_{i=1}^{n}\left|\lambda_{i}\right|^{k}$. Details of the spectral theory of graphs can be found in the seminal monograph [9].

One of the most remarkable chemical application of graph theory is based on the close correspondence between the graph eigenvalues and the molecular orbital energy levels of $\pi$-electrons in conjugated hydrocarbons. In the seventies, Gutman [20] introduced the following definition of graph energy.

Definition 2.1 If $G$ is a graph on $n$ vertices and $\lambda_{1}, \lambda_{2}, \ldots, \lambda_{n}$ are its eigenvalues, then the energy of $G$ is $\mathcal{E}(G)=\sum_{i=1}^{n}\left|\lambda_{i}\right|$.

In the theory of graph energy the so-called Coulson integral formula plays an important role. This formula was obtained by Charles Coulson as early as in 1940 [7], and reads:

$$
\mathcal{E}(G)=\frac{1}{\pi} \int_{-\infty}^{+\infty}\left[n-\frac{i x \phi^{\prime}(G, i x)}{\phi(G, i x)}\right] d x=\frac{1}{\pi} \int_{-\infty}^{+\infty}\left[n-x \frac{d}{d x} \ln \phi(G, i x)\right] d x,
$$

where $G$ is a graph, $\phi(G, x)$ is the characteristic polynomial of $G, \phi^{\prime}(G, x)=$ $(d / d x) \phi(G, x)$ its first derivative, and $i=\sqrt{-1}$. For more details on this useful equality, we refer to [7, 30].

There are two important classes of mathematical problems on graph energy. One class is to find the upper and lower bounds of graph energy. Another relates to determine the extremal values of the energy for a given class of graphs, and also characterize the corresponding extremal graphs. Some of these results are as follows:

For a graph $G$ with $m$ edges, we have $2 \sqrt{m} \leq \mathcal{E}(G) \leq 2 m$ [31]. Let $G$ be a graph with $n$ vertices and $m$ edges. Then $\mathcal{E}(G) \leq \sqrt{2 m n}$ [31]. Koolen
and Moulton [26, 28] obtained the following result: If $2 m \geq n$, then

$$
\mathcal{E}(G) \leq \frac{2 m}{n}+\sqrt{(n-1)\left[2 m-\left(\frac{2 m}{n}\right)^{2}\right]}
$$

If, in addition, $G$ is bipartite, then [27, 28]

$$
\mathcal{E}(G) \leq \frac{4 m}{n}+\sqrt{(n-2)\left[2 m-2\left(\frac{2 m}{n}\right)^{2}\right]}
$$

Let $T$ be a tree of order $n$. A basic result is $\mathcal{E}\left(S_{n}\right) \leq \mathcal{E}(T) \leq \mathcal{E}\left(P_{n}\right)$, see [19]; $S_{n}$ and $P_{n}$ denote the star graph and path graph of order $n$, respectively. The unicyclic graphs with maximum energy are finally determined in [24] and [2], independently. Huo et al. [23] determined the maximal energy among all bipartite bicyclic graphs. Recently, Wagner [42] showed that the maximum value of the graph energy within the set of all graphs with cyclomatic number $k$ (which includes, for instance, trees or unicyclic graphs as special cases) is at most $4 n / \pi+c_{k}$ for some constant $c_{k}$ that only depends on $k$.

For more results on graph energy, we refer to the two surveys [20, 22] and one book [30].

## 3 Generalized graph entropies

Most of the classical graph entropy measures $[4,33]$ are based on an equivalence relation $\tau$ by using a graph invariant $X$ applied to a finite graph. The relation $\tau$ partitions the graph into equivalence classes $X_{i}$ and thus allows defining a probability distribution by using the fact that $[4,6,33]$

$$
\begin{equation*}
\frac{\left|X_{1}\right|+\left|X_{2}\right|+\cdots+\left|X_{k}\right|}{|X|}=1, \tag{1}
\end{equation*}
$$

where $k$ is the number of equivalence classes.
Dehmer [11, 14] introduced another class of graph entropies that is not based on determining partitions induced by equivalence relations using an invariant $X$. To define these measures, a probability value to each vertex $v_{i} \in V$ is assigned, we obtain the following probability distribution

$$
\left(p^{f}\left(v_{1}\right), p^{f}\left(v_{2}\right), \ldots, p^{f}\left(v_{n}\right)\right), \quad|V|:=n,
$$

where

$$
p^{f}\left(v_{i}\right):=\frac{f\left(v_{i}\right)}{\sum_{j=1}^{n} f\left(v_{j}\right)}
$$

and $f$ is an information function mapping graph elements to the non-negative reals, see [11]. The entropy of the underlying graph is

$$
I_{f}(G):=-\sum_{i=1}^{n} \frac{f\left(v_{i}\right)}{\sum_{j=1}^{n} f\left(v_{j}\right)} \log \left(\frac{f\left(v_{i}\right)}{\sum_{j=1}^{n} f\left(v_{j}\right)}\right) .
$$

Actually, following the seminal paper of Shannon [40], many generalizations of the entropy measure have been proposed $[1,10,38]$. An important example of such a measure is called the Rényi entropy [38] and is defined by

$$
I_{\alpha}^{r}(P):=\frac{1}{1-\alpha} \log \left(\sum_{i=1}^{n}\left(p_{i}\right)^{\alpha}\right), \quad \alpha \neq 1,
$$

where $P:=\left(p\left(v_{1}\right), p\left(v_{2}\right), \ldots, p\left(v_{n}\right)\right)$. The limiting value for $\alpha \rightarrow 1$ yields Shannon entropy as a special case.

In [13], Dehmer and Mowshowitz introduced a new class of measures (called here generalized measures) that derive from functions such as those defined by Rényi's entropy [38] and Daròczy's entropy [10].
Definition 3.1 Let $G$ be a graph of order n. Then
(i). $\quad I^{1}(G):=\sum_{i=1}^{n} \frac{f\left(v_{i}\right)}{\sum_{j=1}^{n} f\left(v_{j}\right)}\left[1-\frac{f\left(v_{i}\right)}{\sum_{j=1}^{n} f\left(v_{j}\right)}\right]$,
(ii). $I_{\alpha}^{2}(G):=\frac{1}{1-\alpha} \log \left(\sum_{i=1}^{n}\left(\frac{f\left(v_{i}\right)}{\sum_{j=1}^{n} f\left(v_{j}\right)}\right)^{\alpha}\right), \quad \alpha \neq 1$,
(iii). $\quad I_{\alpha}^{3}(G):=\frac{\sum_{i=1}^{n}\left(\frac{f\left(v_{i}\right)}{\left.\sum_{j=1}^{f f\left(v_{j}\right)}\right)^{\alpha}-1}\right.}{2^{1-\alpha}-1}, \quad \alpha \neq 1$.

Let $G$ be an undirected graph of order $n$ and $A$ its adjacency matrix. Denote by $\lambda_{1}, \lambda_{2}, \ldots, \lambda_{n}$ the eigenvalues of $G$. If $f:=\left|\lambda_{i}\right|$, then [16]

$$
p^{f}\left(v_{i}\right)=\frac{\left|\lambda_{i}\right|}{\sum_{j=1}^{n}\left|\lambda_{i}\right|} .
$$

Therefore, the generalized graph entropies are as follows:

$$
\begin{align*}
& \text { (i). } \quad I^{1}(G):=\sum_{i=1}^{n} \frac{\left|\lambda_{i}\right|}{\sum_{j=1}^{n}\left|\lambda_{i}\right|}\left[1-\frac{\left|\lambda_{i}\right|}{\sum_{j=1}^{n}\left|\lambda_{i}\right|}\right],  \tag{2}\\
& \text { (ii). } \quad I_{\alpha}^{2}(G):=\frac{1}{1-\alpha} \log \left(\sum_{i=1}^{n}\left(\frac{\left|\lambda_{i}\right|}{\sum_{j=1}^{n}\left|\lambda_{i}\right|}\right)^{\alpha}\right), \quad \alpha \neq 1,  \tag{3}\\
& \text { (iii). } \quad I_{\alpha}^{3}(G):=\frac{\sum_{i=1}^{n}\left(\frac{\left|\lambda_{i}\right|}{\sum_{j=1}^{n} \mid \lambda_{i} i}\right)^{\alpha}-1}{2^{1-\alpha}-1}, \quad \alpha \neq 1 . \tag{4}
\end{align*}
$$

## 4 Extremal properties of the generalized graph entropies

In [12], Dehmer and Kraus emphasized that there is a lack of analytical results in the scientific literature when proving extremal results for entropybased graph measures. In this section, we will examine the extremal values of the above stated entropies in terms of graph energy and the spectral moments.

Theorem 4.1 Let $G$ be a graph with $n$ vertices and $m$ edges. Then for $\alpha \neq 1$, we have
(i). $I^{1}(G)=1-\frac{2 m}{\mathcal{E}^{2}}$,
(ii). $\quad I_{\alpha}^{2}(G)=\frac{1}{1-\alpha} \log \frac{M_{\alpha}^{*}}{\mathcal{E}^{\alpha}}$,
(iii). $I_{\alpha}^{3}(G)=\frac{1}{2^{1-\alpha}-1}\left(\frac{M_{\alpha}^{*}}{\mathcal{E}^{\alpha}}-1\right)$,
where $\mathcal{E}$ denotes the energy of graph $G$.
Proof. By substituting $\mathcal{E}=\sum_{i=1}^{n}\left|\lambda_{i}\right|$ into equality (2), we have

$$
\begin{aligned}
I^{1}(G) & =\sum_{i=1}^{n} \frac{\left|\lambda_{i}\right|}{\sum_{j=1}^{n}\left|\lambda_{i}\right|}\left[1-\frac{\left|\lambda_{i}\right|}{\sum_{j=1}^{n}\left|\lambda_{i}\right|}\right] \\
& =\sum_{i=1}^{n} \frac{\left|\lambda_{i}\right|}{\mathcal{E}}\left(1-\frac{\left|\lambda_{i}\right|}{\mathcal{E}}\right)=\frac{1}{\mathcal{E}^{2}} \sum_{i=1}^{n}\left|\lambda_{i}\right|\left(\mathcal{E}-\left|\lambda_{i}\right|\right) \\
& =\frac{1}{\mathcal{E}^{2}}\left(\mathcal{E}^{2}-\sum_{i=1}^{n}\left|\lambda_{i}\right|^{2}\right)=1-\frac{2 m}{\mathcal{E}^{2}}
\end{aligned}
$$

The last equality holds since $\sum_{i=1}^{n} \lambda_{i}^{2}=2 m$.
The other two equalities can be obtained by substituting $\mathcal{E}=\sum_{i=1}^{n}\left|\lambda_{i}\right|$ and $M_{\alpha}^{*}=\sum_{i=1}^{n}\left|\lambda_{i}\right|^{\alpha}$ into equalities (3) and (4), respectively.

From equality (5), we can easily infer the relation of $I^{1}(G)$ and the energy $\mathcal{E}(G)$. Therefore, we have the following two corollaries on $I^{1}(G)$.

Corollary 4.2 For a graph $G$, each upper (lower) bound of energy $\mathcal{E}(G)$ can deduce an upper (a lower) bound of $I^{1}(G)$.

Corollary 4.3 (i). For a graph $G$ with $m$ edges, we have

$$
\frac{1}{2} \leq I^{1}(G) \leq 1-\frac{1}{2 m}
$$

(ii). Let $G$ be a graph with $n$ vertices and $m$ edges. Then

$$
I^{1}(G) \leq 1-\frac{1}{n}
$$

(iii). Let $T$ be a tree of order $n$. We have

$$
I^{1}\left(S_{n}\right) \leq I^{1}(T) \leq I^{1}\left(P_{n}\right)
$$

where $S_{n}$ and $P_{n}$ denote the star graph and path graph of order $n$, respectively.
(iv). Let $G$ be a unicyclic graph of order $n$, then we have

$$
I^{1}(G) \leq I^{1}\left(P_{n}^{6}\right)
$$

where $P_{n}^{6}$ denotes the unicyclic graph obtained by connecting a vertex of $C_{6}$ with a leaf of $P_{n-6}$ (e.g., $P_{14}^{6}$ is shown in Figure 1).
(v). Let $G$ be a graph with cyclomatic number $k$, then we have

$$
I^{1}(G) \leq 1-\frac{2 m}{\left(4 n / \pi+c_{k}\right)^{2}}
$$

where $c_{k}$ is a constant which only depends on $k$.


Figure 1: The graph $P_{14}^{6}$.
In the following part of this section, we present our main results on implicit information inequalities.

Theorem 4.4 (i). When $0<\alpha<1$, we have $I_{\alpha}^{2}<I_{\alpha}^{3} \cdot \ln 2$; and when $\alpha>1$, we have $I_{\alpha}^{2}>\frac{\left(1-2^{1-\alpha}\right) \ln 2}{\alpha-1} I_{\alpha}^{3}$.
(ii). When $\alpha \geq 2$ and $0<\alpha<1$, we have $I_{\alpha}^{3}>I^{1}$; when $1<\alpha<2$, we have $I^{1}>\left(1-2^{1-\alpha}\right) I_{\alpha}^{3}$.
(iii). When $\alpha \geq 2$ and $0<\alpha<1$, we have

$$
I_{\alpha}^{2}>\frac{\left(1-2^{1-\alpha}\right) \ln 2}{\alpha-1} I^{1}
$$

when $1<\alpha<2$, we have

$$
I_{\alpha}^{2}>\frac{\left(1-2^{1-\alpha}\right)^{2} \ln 2}{\alpha-1} I^{1}
$$

when $0<\alpha<1$, we have $I_{\alpha}^{2}>I^{1}$.
Proof. Now we define a new function on $\alpha>0$ as follows,

$$
f(\alpha)=\log \frac{M_{\alpha}^{*}}{\mathcal{E}^{\alpha}}=\log \frac{\left|\lambda_{1}\right|^{\alpha}+\cdots+\left|\lambda_{n}\right|^{\alpha}}{\left(\left|\lambda_{1}\right|+\cdots+\left|\lambda_{n}\right|\right)^{\alpha}}
$$

We claim that $f(\alpha)$ is a monotonously decreasing function on $\alpha$, since

$$
\begin{aligned}
f^{\prime} & =\frac{1}{\ln 2} \cdot \frac{\left|\lambda_{1}\right|^{\alpha} \ln \left|\lambda_{1}\right|+\cdots+\left|\lambda_{n}\right|^{\alpha} \ln \left|\lambda_{n}\right|}{\left|\lambda_{1}\right|^{\alpha}+\cdots+\left|\lambda_{n}\right|^{\alpha}}-\log \left(\left|\lambda_{1}\right|+\cdots+\left|\lambda_{n}\right|\right) \\
& <\frac{\ln \left|\lambda_{\max }\right|}{\ln 2} \cdot \frac{\left|\lambda_{1}\right|^{\alpha}+\cdots+\left|\lambda_{n}\right|^{\alpha}}{\left|\lambda_{1}\right|^{\alpha}+\cdots+\left|\lambda_{n}\right|^{\alpha}}-\log \left(\left|\lambda_{1}\right|+\cdots+\left|\lambda_{n}\right|\right) \\
& =\log \left|\lambda_{\max }\right|-\log \left(\left|\lambda_{1}\right|+\cdots+\left|\lambda_{n}\right|\right)<0,
\end{aligned}
$$

where $\left|\lambda_{\max }\right|=\max \left\{\left|\lambda_{1}\right|, \ldots,\left|\lambda_{n}\right|\right\}$. Therefore, the function $\frac{M_{\alpha}^{*}}{\mathcal{E}^{\alpha}}$ is also a monotonously decreasing function on $\alpha>0$.
(i). Observe that $\alpha>0$ and $\alpha \neq 1$, we have

$$
\frac{M_{\alpha}^{*}}{\mathcal{E}^{\alpha}}=\frac{\sum_{i=1}^{n}\left|\lambda_{i}\right|^{\alpha}}{\left(\sum_{i=1}^{n}\left|\lambda_{i}\right|\right)^{\alpha}} \begin{cases}>1, & 0<\alpha<1 \\ <1, & \alpha>1\end{cases}
$$

and

$$
\log \frac{M_{\alpha}^{*}}{\mathcal{E}^{\alpha}}<\left(\frac{M_{\alpha}^{*}}{\mathcal{E}^{\alpha}}-1\right) \ln 2
$$

By some calculations, we have $\frac{1}{1-\alpha}<\frac{1}{2^{1-\alpha}-1}$ for $0<\alpha<1$ and $\frac{1}{1-\alpha}>$ $\frac{1}{2^{1-\alpha}-1}$ for $\alpha>1$.

Therefore, for $0<\alpha<1$, we have

$$
\frac{1}{1-\alpha} \log \frac{M_{\alpha}^{*}}{\mathcal{E}^{\alpha}}<\frac{\ln 2}{2^{1-\alpha}-1}\left(\frac{M_{\alpha}^{*}}{\mathcal{E}^{\alpha}}-1\right)
$$

For $\alpha>1$, we have

$$
\frac{I_{\alpha}^{2}}{I_{\alpha}^{3}}=\frac{\frac{1}{1-\alpha} \log \frac{M_{\alpha}^{*}}{\mathcal{E}^{\alpha}}}{\frac{1}{2^{1-\alpha}-1}\left(\frac{M_{\alpha}^{*}}{\mathcal{E}^{\alpha}}-1\right)}>\frac{\frac{\ln 2}{1-\alpha}\left(\frac{M_{\alpha}^{*}}{\mathcal{E}^{\alpha}}-1\right)}{\frac{1}{2^{1-\alpha}-1}\left(\frac{M_{\alpha}^{*}}{\mathcal{E}^{\alpha}}-1\right)}=\frac{\left(1-2^{1-\alpha}\right) \ln 2}{\alpha-1}
$$

(ii). For $\alpha \geq 2$, we want to show the following inequality

$$
1-\frac{2 m}{\mathcal{E}^{2}}<\frac{1}{2^{1-\alpha}-1}\left(\frac{M_{\alpha}^{*}}{\mathcal{E}^{\alpha}}-1\right)=\frac{1}{1-2^{1-\alpha}}\left(1-\frac{M_{\alpha}^{*}}{\mathcal{E}^{\alpha}}\right)
$$

i.e.,

$$
\frac{1}{1-2^{1-\alpha}} \frac{M_{\alpha}^{*}}{\mathcal{E}^{\alpha}}-\frac{M_{2}^{*}}{\mathcal{E}^{2}}<\frac{1}{1-2^{1-\alpha}}-1
$$

Since $\frac{M_{\alpha}^{*}}{\mathcal{E}^{\alpha}}$ is decreasing on $\alpha$ and then for $\alpha \geq 2$, we have
$\frac{1}{1-2^{1-\alpha}} \frac{M_{\alpha}^{*}}{\mathcal{E}^{\alpha}}-\frac{M_{2}^{*}}{\mathcal{E}^{2}} \leq \frac{1}{1-2^{1-\alpha}} \frac{M_{2}^{*}}{\mathcal{E}^{2}}-\frac{M_{2}^{*}}{\mathcal{E}^{2}}=\left(\frac{1}{1-2^{1-\alpha}}-1\right) \frac{M_{2}^{*}}{\mathcal{E}^{2}}<\frac{1}{1-2^{1-\alpha}}-1$.
Therefore, the required inequality holds. Similarly, we can prove that for $0<\alpha<1$, we have $I_{\alpha}^{3}>I^{1}$.

Now suppose $1<\alpha<2$, we have $\frac{M_{\alpha}^{*}}{\mathcal{E}^{\alpha}}>\frac{M_{2}^{*}}{\mathcal{E}^{2}}$ and then

$$
\begin{aligned}
I_{\alpha}^{3}-I^{1} & =\frac{1}{1-2^{1-\alpha}}\left(1-\frac{M_{\alpha}^{*}}{\mathcal{E}^{\alpha}}\right)-\left(1-\frac{M_{2}^{*}}{\mathcal{E}^{2}}\right) \\
& <\frac{1}{1-2^{1-\alpha}}\left(1-\frac{M_{2}^{*}}{\mathcal{E}^{2}}\right)-\left(1-\frac{M_{2}^{*}}{\mathcal{E}^{2}}\right) \\
& =\left(\frac{1}{1-2^{1-\alpha}}-1\right)\left(1-\frac{M_{2}^{*}}{\mathcal{E}^{2}}\right)
\end{aligned}
$$

This implies that $I_{\alpha}^{3}-I^{1}<\left(\frac{1}{1-2^{1-\alpha}}-1\right) I^{1}$, i.e., $I^{1}>\left(1-2^{1-\alpha}\right) I_{\alpha}^{3}$.
(iii). From (i) and (ii), we can easily obtain the following results: when $\alpha \geq 2$, we have

$$
I_{\alpha}^{2}>\frac{\left(1-2^{1-\alpha}\right) \ln 2}{\alpha-1} I^{1}
$$

when $1<\alpha<2$, we have

$$
I_{\alpha}^{2}>\frac{\left(1-2^{1-\alpha}\right)^{2} \ln 2}{\alpha-1} I^{1}
$$

By some elementary analysis, we can prove that for $0<\alpha<1$, we have $I_{\alpha}^{2}>I^{1}$.

## 5 Numerical results

In this section, as an example, we compute the exact values of $I^{1}, I_{\alpha}^{2}$ and $I_{\alpha}^{3}$ for the graph $P_{14}^{6}$ as shown in Figure 1. By some calculations, on can obtain the spectrum of the given graph as follows:
$\{ \pm 2.15830, \pm 1.86755, \pm 1.57475, \pm 1.25341, \pm 1.00000, \pm 0.84541, \pm 0.29735\}$.

Therefore, the value of the energy is 17.99354 . Thus, we get

$$
\begin{gathered}
I^{1}=1-\frac{2 m}{\mathcal{E}^{2}}=1-\frac{2 \times 13}{17.99354^{2}}=0.919695 \\
I_{\alpha}^{2}=\frac{1}{1-\alpha} \log \frac{2\left(1+2.15830^{\alpha}+1.86755^{\alpha}+1.57475^{\alpha}+1.25341+0.84541^{\alpha}+0.29735^{\alpha}\right)}{17.99354^{\alpha}}
\end{gathered}
$$

and

$$
\begin{aligned}
I_{\alpha}^{3}= & \frac{1}{2^{1-\alpha}-1} . \\
& \left(\frac{2\left(1+2.15830^{\alpha}+1.86755^{\alpha}+1.57475^{\alpha}+1.25341+0.84541^{\alpha}+0.29735^{\alpha}\right)}{17.99354^{\alpha}}-1\right) .
\end{aligned}
$$



Figure 2: $I_{\alpha}^{2}$ (blue) and $I_{\alpha}^{3}($ red $)$ vs. $\alpha$ (with a pole at $\alpha=1$ ).
From Figure 2, we can see the plotted values of the entropy measures relative to $\alpha$ (with a pole at $\alpha=1$ ).

Now, we will interpret the numerical results, as shown in Figure 2. First we observe that there exists one point $\alpha_{0}$ satisfying that, the value of $I_{\alpha}^{2}\left(P_{14}^{6}\right)$ is always less than that of $I_{\alpha}^{3}\left(P_{14}^{6}\right)$ for $0<\alpha<\alpha_{0}$, while the value of $I_{\alpha}^{2}\left(P_{14}^{6}\right)$ is always larger than that of $I_{\alpha}^{3}\left(P_{14}^{6}\right)$ for $0<\alpha>\alpha_{0}$. From Figure 2, we can see that the value of $\alpha_{0}$ is about 1.4667. For $I^{1}\left(P_{14}^{6}\right)$ and $I_{\alpha}^{2}\left(P_{14}^{6}\right)$, we can see that the value of $I_{\alpha}^{2}\left(P_{14}^{6}\right)$ is always larger than that of $I^{1}\left(P_{14}^{6}\right)$ for any $\alpha>0$. On the other hand, observe that the value of $I_{\alpha}^{3}\left(P_{14}^{6}\right)$ is a decreasing function on $\alpha$. Actually, some elementary calculations show that the value of $I_{\alpha}^{3}\left(P_{14}^{6}\right)$ tends to 1 when $\alpha$ tends to $+\infty$. Therefore, we can also obtain that the value of $I_{\alpha}^{3}\left(P_{14}^{6}\right)$ is always larger than that of $I^{1}\left(P_{14}^{6}\right)$ for any $\alpha>0$. These observations verify our inequalities in Theorem 4.4.

## 6 Summary and conclusion

In this paper, we studied the generalized graph entropies, which was introduced by Dehmer and Mowshowitz in [13] and derive from functions such as those defined by Rényi's entropy [38] and Daròczy's entropy [10]. As reported in [12], there is a lack of analytical results in the scientific literature when proving extremal results for entropy-based graph measures. We examined the extremal values of the above stated entropies in terms of graph energy and the spectral moments. We also proved some inequalities between these generalized graph entropies. As a future work, we want to explore general methods to show the extremal values of other graph entropy measures for characterizing the structural complexity of graphs.

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