Research Article

Some New Bounds of Weighted Graph Entropies with GA and Gaurava Indices Edge Weights

Tiejun Wu,¹ Hafiz Mutee Ur Rehman ,^{2,3} Yu-Ming Chu ,^{4,5} Deeba Afzal,² and Jianfeng Yu¹

¹College of Mechanical and Electronics Engineering, Dongguan Polytechnic, Dongguan 523808, Guangdong, China

²Department of Mathematics and Statistics, The University of Lahore, Lahore, Pakistan

³Department of Mathematics, Division of Science and Technology, University of Education, Lahore, Pakistan

⁴Department of Mathematics, Huzhou University, Huzhou 313000, China

⁵Hunan Provincial Key Laboratory of Mathematical Modeling and Analysis in Engineering, Changsha University of Science & Technology, Changsha 410114, China

Correspondence should be addressed to Yu-Ming Chu; chuyuming@zjhu.edu.cn

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Motivated by the concept of Shannon's entropy, the degree-dependent weighted graph entropy was defined which is now become a tool for measurement of structural information of complex graph networks. The aim of this paper is to study weighted graph entropy. We used GA and Gaurava indices as edge weights to define weighted graph entropy and establish some bounds for different families of graphs. Moreover, we compute the defined weighted entropies for molecular graphs of some dendrimer structures.

1. Introduction

The branch of mathematics known as graph theory provides tools for solving problems of information theory, computer sciences, physics, and chemistry [1–3]. Among them, special places are reserved for so-called topological descriptors, which play an important role in mathematical chemistry, especially in QSPR/QSAR surveys. Many topological descriptors are introduced and studied in the literature, such as the Zagreb index [4–6], the Randić connectivity index [7], and the modified Zagreb index [8, 9].

In the year 2009, Vukičević and Furtula [10] introduced the geometrical arithmetic (GA) index as a molecular descriptor, and mathematical formula for this index is,

$$GA_1 = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}. \quad (1)$$

There are many interesting attributes on topological indices, and different physicochemical properties of

hydrocarbons can be obtained from this index [11–16]. The predictive power of the GA index is compared with others such as the famous Randić index [17]. Due to this reason, different versions of the GA index are now investigated and introduced in the literature [18–20]. The other famous indices are given in [21]. The mathematical formulae for first and second Gaurava indices are

$$GO_1 = \sum_{uv \in E(G)} [(d_u + d_v) + (d_u \cdot d_v)], \quad (2)$$

$$GO_2 = \sum_{uv \in E(G)} [(d_u + d_v) \cdot (d_u \cdot d_v)], \quad (3)$$

respectively.

Many problems of information theory, biology, computer sciences, chemistry, and discrete mathematics are directly solved by utilizing different kinds of graph measures and the graph entropy is one of the powerful tools [22–26] that help to understand the structural

complexity of graph networks [27]. Different molecular descriptors are used to introduce weighted graph entropies [28–31].

In this paper, we extended the work of [28, 30] and introduced weighted graph entropies by using GA and Gaurava indices as edge weights. We examine the extreme properties of these entropies for some special graph families. We also computed these entropies for different chemical structures.

Now, we define some basic notions about entropy of graphs. We always consider G being a connected graph with E as the set of edges, V as the set of vertices, and w to be the edge weight given to the edges of graph G that will be used to define weighted graph entropy. As mentioned above, GA and Gaurava indices are taken as edge weights in this paper. d_u denoted the degree of a vertex u that is defined as the total number of vertices of G that are at distance one from the vertex u . Consider

$$p_{ij} = \frac{w(v_i v_j)}{\sum_{j=1} d_i w(v_i v_j)}, \quad (4)$$

where $w(v_i v_j)$ is the weight $v_i v_j$ and $w(v_i v_j) > 0$.

Now, the weighted graph entropy can be defined by

$$H(v_i) = - \sum p_{ij} \log(p_{ij}). \quad (5)$$

Definition 1. For the graph G , the weighted entropy can be defined as follows [28, 30]:

$$I(G, w) = - \sum_{uv \in E(G)} p_{uv} \log(p_{uv}). \quad (6)$$

Here, p_{uv} is same as that given in (4).

2. Main Results

In this section, we are going to present our main results.

Lemma 1. Let G be a simple graph having n vertices and m edges and let Δ and δ be the maximum degree and minimum degree of a vertex, respectively; then,

$$\begin{aligned} & \frac{2\nu\sqrt{\Delta}}{\Delta+1} + \sqrt{\mu^2 - \frac{\mu}{4\delta_1^2} \left[\sum_1 d_i^3 - 2M_2(G) - \nu(\delta_1 - 1)^2 \right] - \frac{\mu^2}{4} \left(1 - \frac{2\sqrt{\Delta}\delta_1}{\Delta+1} \right)^2} \\ & \leq GA_1 \leq \frac{2\nu\sqrt{\delta_1}}{\delta_1+1} + \sqrt{\mu^2 - \frac{\mu}{4\Delta^2} \left[\sum_1 d_i^3 - 2M_2(G) - \nu(\Delta - 1)^2 \right]}, \end{aligned} \quad (7)$$

with equality if and only if G is a regular graph or G is a bipartite graph.

Lemma 2. Consider G is a simple connected graph having m edges. Then, we have

$$GA_1 \leq \frac{2\nu\sqrt{\Delta}}{\Delta+1} + \frac{1}{\Delta} \sqrt{M_2(G) - \nu\Delta + (m - \nu)\delta_1^2}, \quad (8)$$

with equality if and only if G is isomorphic to $K_{1,n-1}$ or G is isomorphic to regular graph or G is isomorphic to $(\Delta, 1)$ semiregular graph.

Lemma 3. Consider G is a simple connected graph having m edges. Then, we have

$$GA_1 \geq \frac{2\nu\sqrt{\Delta}}{\Delta+1} \frac{8\sqrt{(\Delta+\delta_1)(\Delta\delta_1)}}{(\sqrt{\delta} + \sqrt{\Delta})^2} \sqrt{(m - \nu)^2 \left(\frac{m - \nu}{4\delta_1^2} \right) \left[\sum_1 d_i^3 - 2M_2(G) - \nu(\delta_1 - 1)^2 \right]}. \quad (9)$$

Moreover, the equality holds if and only if G is isomorphic to a regular graph or G is isomorphic to $(\Delta, 1)$ semiregular graph.

Lemma 4. Consider G is a simple connected graph having m edges. Then, we have

$$GA_1 \leq \frac{2m\sqrt{2}(n-1)}{n+1} - 2\nu \left(\frac{\sqrt{2(n-1)}}{n+1} - \frac{\sqrt{n-1}}{n} \right), \quad (10)$$

with equality if and only if G is isomorphic to $K_{1,n-1}$ or G is isomorphic to a complete graph K_3 .

Lemma 5. Consider G is a simple connected graph having m edges. Then, we have

$$GA_1 \leq \left\lceil \frac{m-1}{n-1} \right\rceil + \sqrt{\left\lceil \frac{m-1}{n-1} \right\rceil^2 + \frac{M_2(G)}{n-1}}. \quad (11)$$

Theorem 1. Consider G is a connected graph having n vertices with $n \geq 3$. Then, we have

$$\begin{aligned} \log(GA_1) + \log\left(\frac{2}{n}\right) &\leq I(G, GA_1) \leq \log(GA_1) \\ &+ \log\left(\frac{n}{4}\right); \end{aligned} \quad (12)$$

$$\begin{aligned} \log(GO_1) + \log 4(n-1) &\leq I(G, GO_1) \leq \log(GO_1) \\ &- \log(3(n-1)^2). \end{aligned}$$

Proof. We prove the result for GO_1 , the other results can be proved in the same manner.

Since G is a connected graph with n number of vertices, for any vertex, the maximum possible degree can be $n-1$ and the minimum possible degree can be one. Hence, for any edge uv , the minimum degrees for u and v can be 1 and 2 and maximum possible degrees for u and v can be $n-1$ and $n-1$, and hence, we have

$$\begin{aligned} I(G, GO_1) &= \log(GO_1) - \frac{1}{GO_1} \sum_{uv \in E(G)} [(d_u + d_v) + (d_u \cdot d_v)] \cdot \log \left[\sum_{uv \in E(G)} (d_u + d_v) + (d_u \cdot d_v) \right] \\ &\leq \log(GO_1) - [\log(3) + \log(n-1)^2] \\ &= \log(GO_1) - \log(3(n-1)^2) \\ &\geq \log(GO_1) - \frac{1}{GO_1} \sum_{uv \in E(G)} [(d_u + d_v) + (d_u \cdot d_v)] \cdot \log \left[\sum_{uv \in E(G)} (d_u + d_v) + (d_u \cdot d_v) \right] \\ &\geq \log(GO_1) - [\log 2(n-2) + \log(2)] \\ &= \log(GO_1) + \log(4n-1). \end{aligned} \quad (13)$$

Therefore,

$$\begin{aligned} \log(GO_1) + \log 4(n-1) &\leq I(G, GO_1) \leq \log(GO_1) \\ &- \log(3(n-1)^2). \end{aligned} \quad (14)$$

□

Theorem 2. Let G be a graph with n vertices. Let δ and Δ be the minimum and maximum degrees of G , respectively. Then, we have

$$\begin{aligned} \log(GA_1) + \log\left(\frac{\delta}{\Delta}\right) &\leq I(G, GA_1) \\ \log(GO_1) - \log(2\Delta\delta^2) &\geq I(G, ReZ_1) \\ &\geq \log(GO_1) - \log(2\delta\Delta^2). \end{aligned} \quad (15)$$

Proof. Since G is the connected graph with n number of vertices, for any vertex, the maximum possible degree can be $n-1$ and the minimum possible degree can be one. Hence, for any edge uv , the minimum degrees for u and v can be 1

and 2 and maximum possible degrees for u and v can be $n-1$ and $n-1$, and hence, we have

$$\begin{aligned} I(G, GO_1) &= \log(GO_1) - \frac{1}{GO_1} \sum_{uv \in E(G)} [(d_u + d_v) + (d_u \cdot d_v)] \\ &\cdot \log \left[\sum_{uv \in E(G)} (d_u + d_v) + (d_u \cdot d_v) \right] \\ &= \log(GO_1) - \frac{1}{GO_1} \sum_{uv \in E(G)} (d_u + d_v) + (d_u \cdot d_v) \\ &\cdot [\log(d_u + d_v) + \log(d_u \cdot d_v)] \\ &= \log(GO_1) - \log(2\Delta\delta^2). \end{aligned} \quad (16)$$

Also,

$$I(G, GO_1) \geq \log(GO_1) - \log(2\delta\Delta^2). \quad (17)$$

□

Theorem 3. Consider G is a regular graph having n vertices with $n \geq 3$. Then, we have

$$\log(n) \leq I(G, GA_1) \leq \log\left(\frac{n(n-1)}{2}\right). \quad (18)$$

Note that left inequality turns into equality if G is a cyclic graph, and the right inequality turns into equality if G is a complete graph.

Theorem 4. Consider G is a complete bipartite graph having n vertices. Then, we have

$$\log(n-1) \leq I(G, GA_1) \leq \log\left(\left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil\right). \quad (19)$$

Note that the left inequality turns into equality if G is a star graph, and $\log(n-1) = \log(\lfloor n/2 \rfloor \lceil n/2 \rceil)$ if and only if G is a complete bipartite graph (balanced).

Theorem 5. Let T be a tree of order $n(n > 2)$ with maximum degree vertex Δ ; then, we have

$$\log(GA_1) \leq \log\left(\frac{2p\sqrt{\Delta}}{\Delta+1}\right). \quad (20)$$

Theorem 6. Let G be a simple graph having n vertices and m edges and let Δ and δ be the maximum degree and minimum degree of a vertex, respectively; then,

$$\log\left(\frac{2m\sqrt{\delta \cdot \Delta}}{\delta + \Delta}\right) \leq I(G, GA_1), \quad (21)$$

with equality if and only if G is either a regular graph or a bipartite graph.

In graph theory, the molecular graph is obtained by taking atoms as vertices and bonds as edges. It can be noted that the maximum possible degree for a vertex in a molecular graph is four. Following theorem is about the bounds of weighted entropy for the molecular graph.

Theorem 7. Consider a molecular graph G having n vertices. Then, we have

$$\log(GA_1) - \log 4 \leq I(G, GA_1) \leq \log(GA_1) + \log\sqrt{2}. \quad (22)$$

2.1. Relation of Entropy with Zagreb Indices

Theorem 8. Consider G is a simple connected graph. Then, we have

$$\log\left(\frac{2M_1(G)}{n(n-1)}\right) \leq I(G, GA_1) \leq \log(M_1(G))^2. \quad (23)$$

The equality holds if and only if G is a union of K_2 .

Theorem 9. Consider G is any graph, then we have

$$I(G, GA_1) \geq \log\left(\frac{2\sqrt{mM_2(G)}}{(n-1)}\right). \quad (24)$$

Equality holds if and only if G is isomorphic to the regular graph.

Theorem 10. Consider G is any graph, then we have

$$\log\left(\frac{2\sqrt{mM_2(G) + m(m-1)}}{(n-1)}\right) \leq I(G, GA_1). \quad (25)$$

Equality holds if and only if G is isomorphic to the regular graph.

Theorem 11. Consider G is any graph, then we have

$$I(G, GA_1) \leq \log\left(\frac{4(n-1)^2\nu\sqrt{\Delta}}{\Delta+1} + \frac{2(n-1)}{\Delta} \cdot \sqrt{M_2(G) - \nu\Delta + (m-\nu)\delta_1^2}\right). \quad (26)$$

Equality holds if and only if G is isomorphic to the regular graph.

2.2. Numerical Examples. Here, we compute the weighted entropies introduced in this paper for some chemical structures.

Example 1. Consider the porphyrin dendrimers shown in Figure 1. We denote the graph of porphyrin dendrimers by G , and the edge partition of G is given in Table 1. Using Table 1 and definition of entropy,

FIGURE 1: Porphyrin dendrimer.

TABLE 1: Edge partition of porphyrin dendrimers.

(d_u, d_v)	(1, 3)	(1, 4)	(2, 2)	(2, 3)	(3, 3)	(3, 4)
Number of edges	$2n$	$24n$	$10n - 5$	$48n - 6$	$13n -$	$8n -$

we have the following entropies for porphyrin dendrimers:

$$\begin{aligned}
 I(G, GA_1) &= \log(GA_1) - \frac{1}{GA_1} \sum_{uv \in E(G)} 2 \frac{\sqrt{d_u d_v}}{d_u \cdot d_v} \cdot \log \left(2 \frac{\sqrt{d_u d_v}}{d_u \cdot d_v} \right) \\
 &= \log(98.88020n - 10.87877) - \frac{1}{98.88020n - 10.87877} \left[|E_1| \left(2 \frac{\sqrt{3}}{4} \cdot \log \left(2 \frac{\sqrt{3}}{4} \right) \right) \right. \\
 &\quad + |E_2| \left(2 \frac{\sqrt{4}}{5} \cdot \log \left(2 \frac{\sqrt{4}}{5} \right) \right) + |E_3| \left(2 \frac{\sqrt{4}}{4} \cdot \log \left(2 \frac{\sqrt{4}}{4} \right) \right) + |E_4| \left(2 \frac{\sqrt{6}}{4} \cdot \log \left(2 \frac{\sqrt{6}}{4} \right) \right) \\
 &\quad + |E_5| \left(2 \frac{\sqrt{6}}{6} \cdot \log \left(2 \frac{\sqrt{6}}{6} \right) \right) + |E_7| \left(2 \frac{\sqrt{12}}{7} \cdot \log \left(2 \frac{\sqrt{12}}{7} \right) \right) \Big] \\
 &= \log(98.88020n - 10.87877) - \frac{1}{98.88020n - 10.87877} \left[(2n) \left(2 \frac{\sqrt{3}}{4} \cdot \log \left(2 \frac{\sqrt{3}}{4} \right) \right) \right. \\
 &\quad + (24n) \left(2 \frac{\sqrt{4}}{5} \cdot \log \left(2 \frac{\sqrt{4}}{5} \right) \right) + (10n - 5) \left(2 \frac{\sqrt{4}}{4} \cdot \log \left(2 \frac{\sqrt{4}}{4} \right) \right) + (48n - 6) \left(2 \frac{\sqrt{6}}{5} \cdot \log \left(2 \frac{\sqrt{6}}{5} \right) \right) \\
 &\quad + (13n) \left(2 \frac{\sqrt{6}}{6} \cdot \log \left(2 \frac{\sqrt{6}}{6} \right) \right) + (8n) \left(2 \frac{\sqrt{12}}{7} \cdot \log \left(2 \frac{\sqrt{12}}{7} \right) \right) \Big], \\
 I(G, GA_1) &= \log(GA_1) - \frac{1}{GA_1} (-23.308n - 2.695),
 \end{aligned} \tag{27}$$

$$\begin{aligned}
I(G, GO_1) &= \log(GO_1) - \frac{1}{GO_1} \sum_{uv \in E(G)} [(d_u + d_v) + (d_u \cdot d_v)] \cdot \log \left[\sum_{uv \in E(G)} (d_u + d_v) + (d_u \cdot d_v) \right] \\
&= \log(1169n - 106) - \frac{1}{1169n - 106} \left[|E_1| [(1+3) + (1.3)] \cdot \log[(1+3) + (1.3)] \right. \\
&\quad + |E_2| [(1+4) + (1.4)] \cdot \log[(1+4) + (1.4)] + |E_3| [(2+2) + (2.2)] \cdot \log[(2+2) + (2.2)] \\
&\quad + |E_4| [(2+3) + (2.3)] \cdot \log[(2+3) + (2.3)] + |E_5| [(3+3) + (3.3)] \cdot \log[(3+3) + (3.3)] \\
&\quad \left. + |E_6| [(3+4) + (3.4)] \cdot \log[(3+4) + (3.4)] \right] \\
&= \log(1169n - 106) - \frac{1}{1169n - 106} [(14n) \cdot \log[7]] \\
&\quad + |E_2| [(1+4) + (1.4)] \cdot \log[(1+4) + (1.4)] + |E_3| [(2+2) + (2.2)] \cdot \log[(2+2) + (2.2)] \\
&\quad + |E_4| [(2+3) + (2.3)] \cdot \log[(2+3) + (2.3)] + |E_5| [(3+3) + (3.3)] \cdot \log[(3+3) + (3.3)] \\
&\quad + |E_6| [(3+4) + (3.4)] \cdot \log[(3+4) + (3.4)], \\
I(G, GO_1) &= \log(GA_1) - \frac{1}{GA_1} (-23.308n - 2.695),
\end{aligned} \tag{28}$$

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is given in Table 2. We have the following computations for the entropies of zinc-porphyrin dendrimer.

Example 2. The graph G of zinc-porphyrin dendrimer is shown in Figure 2, and the edge partition for this dendrimer

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$$\begin{aligned}
I(G, GA_1) &= \log(GA_1) - \frac{1}{GA_1} \sum_{uv \in E(G)} 2 \frac{\sqrt{d_u d_v}}{d_u \cdot d_v} \cdot \log \left(2 \frac{\sqrt{d_u d_v}}{d_u \cdot d_v} \right) \\
&= \log(44.9312^n - 22.226) - \frac{1}{2(44.9312^n - 22.226)} \left[|E_1| \left(\frac{\sqrt{2}}{2} \right) \cdot \log \left(\frac{\sqrt{2}}{2} \right) \right. \\
&\quad + |E_2| \left(\frac{\sqrt{2}}{2} \right) \cdot \log \left(\frac{\sqrt{2}}{2} \right) + |E_3| \left(\frac{2}{3} \right) \cdot \log \left(\frac{2}{3} \right) + |E_4| \left(\frac{\sqrt{15}}{6} \right) \cdot \log \left(\frac{\sqrt{15}}{6} \right) \\
&= \log(44.9312^n - 22.226) - \frac{1}{2(44.9312^n - 22.226)} \left[(16.2^n - 4) \left(\frac{\sqrt{2}}{2} \right) \cdot \log \left(\frac{\sqrt{2}}{2} \right) \right. \\
&\quad \left. + (40.2^n - 16) \left(\frac{\sqrt{2}}{2} \right) \cdot \log \left(\frac{\sqrt{2}}{2} \right) + (8.2^n - 16) \left(\frac{2}{3} \right) \cdot \log \left(\frac{2}{3} \right) + (4) \left(\frac{\sqrt{15}}{6} \right) \cdot \log \left(\frac{\sqrt{15}}{6} \right) \right].
\end{aligned} \tag{29}$$

FIGURE 2: Zinc-porphyrin dendrimer.

TABLE 2: Edge partition of zinc-porphyrin dendrimers.

(d_u, d_v)	(2, 2)	(2, 3)	(3, 3)	(3, 4)
Number of edges	$16 \cdot 2^n - 4$	$40 \cdot 2^n - 16$	$8 \cdot 2^n - 16$	4

FIGURE 3: Poly(ethylene amidoamine) dendrimer.

TABLE 3: Edge partition of the poly(ethylene amidoamine) dendrimer.

(d_u, d_v)	(1, 2)	(1, 3)	(2, 2)	(2, 3)
Number of edges	$4 \cdot 2^n$	$4 \cdot 2^n - 2$	$16 \cdot 2^n$	$20 \cdot 2^n - 9$

Example 3. Let G be the graph of poly(ethylene amido-amine) dendrimers as shown in Figure 3. Then, the edge

partition of this dendrimer is given in Table 3 and we have the following results.

$$\begin{aligned}
 I(G, GA_1) &= \log(GA_1) - \frac{1}{GA_1} \sum_{uv \in E(G)} 2 \frac{\sqrt{d_u d_v}}{d_u \cdot d_v} \cdot \log\left(2 \frac{\sqrt{d_u d_v}}{d_u \cdot d_v}\right) \\
 &= \log(31.5502^n - 13.653) - \frac{1}{2(31.5502^n - 13.653)} \left[|E_1| \left(\frac{\sqrt{2}}{2}\right) \cdot \log\left(\frac{\sqrt{2}}{2}\right) \right. \\
 &\quad \left. + |E_2| \left(\frac{\sqrt{6}}{3}\right) \cdot \log\left(\frac{\sqrt{6}}{3}\right) + |E_3| \left(\frac{2}{2}\right) \cdot \log\left(\frac{2}{2}\right) + |E_4| \left(\frac{\sqrt{2}}{2}\right) \cdot \log\left(\frac{\sqrt{2}}{2}\right) \right] \\
 &= \log(31.5502^n - 13.653) - \frac{1}{2(31.5502^n - 13.653)} \left[(4.2^n) \left(\frac{\sqrt{2}}{2}\right) \cdot \log\left(\frac{\sqrt{2}}{2}\right) \right. \\
 &\quad \left. + (4.2^n - 2) \left(\frac{\sqrt{6}}{3}\right) \cdot \log\left(\frac{\sqrt{6}}{3}\right) + (16.2^n) \left(\frac{2}{2}\right) \cdot \log\left(\frac{2}{2}\right) + (20.2^n - 9) \left(\frac{\sqrt{2}}{2}\right) \cdot \log\left(\frac{\sqrt{2}}{2}\right) \right].
 \end{aligned} \tag{30}$$

3. Conclusion

In information theory, the graph entropy is a measure of the information rate achievable by communicating symbols over a channel in which certain pairs of values may be confused. This measure, first introduced by Körner in the 1970s, has since also proven itself useful in other settings, including combinatorics. In this paper, we have studied graph entropy with GA and Gaurava indices and justified it by some numerical examples. It would be interesting to work on entropy of weighted graphs with some other degree- and distance-based topological indices. The bounds of degree-based network entropy can also be used in national security, Internet networks, social networks, structural chemistry, ecological networks, computational systems biology, etc. They will play an important role in analyzing structural symmetry and asymmetry in real networks in the future.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that they do not have any conflicts of interest.

Authors' Contributions

Tiejun Wu enhanced the introduction section and improved the reference list. Hafiz Mutee Ur Rehman wrote the original paper. Yu-Ming Chu gave the equality conditions for Theorems 1, 2, and 7 and verified all results. Deebea Afzal supervised the work and Jianfeng Yu prepared the revision and arranged funding for the paper.

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