FULL PAPER

Weighted entropy of Zig-Zag chain

Farkhanda Afzal*a, | Sidra Razaqa | Mehmoona Abdul Razaq | Murat Cancan | Mehmet Serif Aldemire

*aMCS, National University of Sciences and Technology, Islamabad, Pakistan
bDepartment of Mathematics, Lahore College for Women University, Jhang Campus, Jhang, Pakistan
cDepartment of Mathematics and Statistics, The University of Lahore, Lahore, Pakistan
dFaculty of Education, Van Yüzüncü Yıl University, Van, Turkey
eFaculty of Science, Van Yüzüncü Yıl University, Van, Turkey

*Corresponding Author:
Farkhanda Afzal
E-mail: farkhanda@mcs.edu.pk
Tel.: +92-3310046177

The entropy of a graph is a functional depending both on the graph itself and on a probability distribution on its vertex set. This graph functional originated from the problem of source coding in information theory and was introduced by J. Krner in 1973. Although the notion of graph entropy has its roots in information theory, it was proved to be closely related to some classical and frequently studied graph theoretic concepts. In this article, we obtained the graph entropy with Randić, geometric-arithmetic, harmonic, first Zagreb, second Zagreb, atom bond connectivity, sum connectivity index and augmented Zagreb indices for Zig-Zag chain of 8-cycles molecular graph.

KEYWORDS
Topological indices; weighted entropy; Zig-Zag chain of 8-cycles.

Introduction

In medicine mathematical model, the structure of drug is represented as an undirected graph, where each vertex indicates an atom and each edge represents a chemical bond between these atoms. With prompt flourishment of manufacturing industry of medicine, hundreds and thousands of drug are produced into market every year. Hence the categorization of the biological, chemical, biochemical and pharmaceutical characteristics of these calls requires a mammoth sum of work, so this work burden has made the data and information more fastidious and clustered. To tryout the benits, performance and side effects of latest and former drugs requires a large gigantic amount of reagents, apparatus and collaboration. However, in developing and poor countries (like Pakistan, India and Africa), it is arduous to manage the expenditures and cost for appliances and reagents required for testing biochemical characteristics. By good luck, previous studies [1, 3-5] have directed the pharmacodynamic and pharmacokinetic properties of drugs and linked information of their chemical composition. It will be helpful for pharmaceutical and medical intellects to know the characteristics of medicine. It will reduce the defects of chemical experiments, if we calculate indicators of these drug molecular structure [2, 6-8] in view of defining the topological indices. For more study and research readers can see [9-26].

Some important formulas of degree based topological indices are given below:

Randić index $R(G)=\sum_{gh\in E(G)} \frac{1}{\sqrt{d_g d_h}}$

Reciprocal Randić index

$RR(G)=\sum_{gh\in E(G)} \frac{1}{\sqrt{d_g d_h}}$

First Zagreb index $M_1(G)=\sum_{gh\in E(G)} (d_g + d_h)$
Second Zagreb index $M_2(G) = \sum_{gh \in E(G)} (d_g \cdot d_h)$

Atom-bond connectivity index $\text{ABC}(G) = \sum_{gh \in E(G)} \sqrt{\frac{d_g + d_h - 2}{d_g \cdot d_h}}$

Augmented Zagreb index $\text{AZI}(G) = \sum_{gh \in E(G)} \left( \frac{d_g \cdot d_h}{d_g + d_h - 2} \right)^2$

Geometric arithmetic index $\text{GA}(G) = \sum_{gh \in E(G)} \frac{2}{d_g + d_h}$

Harmonic index $\text{HI}(G) = \sum_{gh \in E(G)} \frac{1}{d_g + d_h}$

Sum connectivity index $\text{SCI}(G) = \sum_{gh \in E(G)} \frac{1}{\sqrt{d_g + d_h}}$

### Entropy

The entropy of a graph is a functional depending both on the graph itself and on a probability distribution on its vertex set. This graph functional originated from the problem of source coding in information theory and was introduced by J. Krner in 1973. Although the notion of graph entropy has its roots in information theory, it was proved to be closely related to some classical and frequently studied graph theoretic concepts. For example, it provides an equivalent definition for a graph to be perfect and it can also be applied to obtain lower bounds in graph covering problems.

**Definition 1.**

Let the probability density function $P_g = \frac{w(\text{uv})}{\sum W(\text{uv})}$, then the entropy of graph $G$ is defined as

$I(G, w) = \sum P_g \log P_g$.

**Generalization of Zig-Zag chain graph**

For $Z_0(n)$, for $n \geq 1$, $a=2n$ then the number of edges with end degrees $(2,2)$ is $6n+4$, the number of edges with end degrees $(2,3)$ is $4n$, the number of edges with end degrees $(3,3)$ is $4n-3$, total number of edges for any $n$ is given by $14n+1$. It can be observed from Figure 1 that there are following three types of edges

**Theorem 1.** For the Zig-Zag chain, the weighted entropy with Randić index weight is

$$I(Z_0(n), R) = \log(5.9663264952n + 1) + 0.4894192028 \cdot \frac{0.0209406468}{n} + 2.174609452n.$$  

**Proof.** Using the values in Table 1 and then putting the values in definition of Randić index, we have

$R(Z_0(n)) = 5.9663264952n + 1$

$I(Z_0(n), R) = \log(R(n)) \cdot \frac{1}{R(n)} \sum \left( \frac{1}{\sqrt{d_g + d_h}} \log \frac{1}{\sqrt{d_g + d_h}} \right)$

$$= \log(5.9663264952n + 1) - \frac{1}{\sqrt{2.2} \log \frac{1}{\sqrt{2.2}} + 4n \log \frac{1}{\sqrt{2.3}} + (4n - 3) \log \frac{1}{\sqrt{3.3}} + 3.3 \log \frac{1}{\sqrt{3.3}})}$$

$$= \log(5.9663264952n + 1) - \frac{0.167607321}{n} - \frac{0.6353578352}{n} - \frac{0.636161673}{n} + 0.4771212548$$

$$= \log(5.9663265n + 1) - \frac{0.1249387372}{n} + 0.4894192028 \cdot \frac{0.0209406468}{n} + 2.174609452n.$$

**Figure 1.** Zig-Zag Chain ($Z_0(n)$)

**Table 1.** Edge partition of of zig-zag chain

<table>
<thead>
<tr>
<th>Edge</th>
<th>Vertices frequencies</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(d_g(g);d_h(h))$</td>
<td>6$n$+4</td>
</tr>
<tr>
<td>$(2,2)$</td>
<td>4$n$</td>
</tr>
<tr>
<td>$(2,3)$</td>
<td>4$n$</td>
</tr>
<tr>
<td>$(3,3)$</td>
<td>4$n$-3</td>
</tr>
</tbody>
</table>
Theorem 2. For Zig-Zag chain, the weighted Entropy with reciprocal Randić index is

\[ I(Z_n, RR) = \log(33.7979589711n - 1) - 2.2749269537 \]

\[ + \frac{0.0557977874}{n} + 13.1499620172n. \]

Proof. Using the values in Table 1 and then putting the values in definition of reciprocal Randić index, we have

\[ RR(Z_n, RR) = \log(33.7979589711n - 1) - \frac{1}{\sqrt{3}} \sum_{i=1}^{n} (d_i^2 \log(d_i^2)). \]

Theorem 3. For Zig-Zag chain, the weighted entropy with Zagreb indices weight is

\[ I(Z_n, M) = \log(68n - 2) + 2.8795941154 \]

\[ + \frac{0.0643200389}{n} + 23.5522349439n. \]

Proof. Using the values in Table 1 and then putting the values in definition of Zagreb indices, we have

\[ \log(68n - 2) - \frac{1}{M_{ij}} \sum_{i<j} (d_i - d_j)(\log(d_i - d_j)). \]

Theorem 4. For Zig-Zag chain, the weighted entropy with atom-bond connectivity index weight is

\[ I(Z_n, ABC) = \log(9.7377344785n + 0.8284271247) \]

\[ + \frac{0.074991269}{n} + 1.851552166n. \]

Proof. Using the values in Table 1 and then putting the values in definition atom-bond connectivity index, we have

\[ \log(9.7377344785n + 0.8284271247) \]

\[ - \frac{1}{n} \sum_{i<j} \left( \frac{d_i + d_j - 2}{d_i d_j} \right) \log \left( \frac{d_i + d_j - 2}{d_i d_j} \right). \]

Theorem 5. For Zig-Zag chain, the weighted entropy with augmented Zagreb index weight is
\[ I(Z_s, AZI) = \log(125.5625n - 2.171875) + 55.4708179248 + \frac{0.0573844335}{n} - 3.3175626475n. \]

**Proof.** Using the values in Table 1 and then putting the values in definition of augmented Zagreb index, we have

\[
AZI(Z_s) = 125.5625n - 2.171875I(Z_s, AZI)
= \log(AZI) - \frac{1}{AZI} \sum_{v \in V} \left( \left( \frac{d_v}{d_v + d_v - 2} \right)^2 \log \left( \frac{d_v}{d_v + d_v - 2} \right) \right)
= \log(125.5625n - 2.171875) \left( 6(n + 4)(2)^n \log(2)^n + 4n(2)^n \log(2)^n + (4n - 3)(2.25)^n \log(2.25)^n \right)

= \log(125.5625n - 2.171875) - \frac{0.0024959184(64n + 4)(2)^n \log(2)^n + 4n(2)^n \log(2)^n + (4n - 3)(2.25)^n \log(2.25)^n}{n}

\]

**Theorem 6.** For Zig-Zag chain, the weighted entropy with geometric-arithmetic index weight is

\[ I(Z_s, GA) = \log(GA) - \frac{1}{GA} \sum_{v \in V} \left( \frac{d_v}{d_v + d_v - 2} \right)^2 \log \left( \frac{d_v}{d_v + d_v - 2} \right) \]

\[ = \log(13.9191835885n + 1) - \frac{1}{13.9191835885n + 1} \left( 6(n + 4)(2)^n \log(2)^n + 4n(2)^n \log(2)^n + (4n - 3)(2.25)^n \log(2.25)^n \right) \]

**Proof.** Using the values in Table 1 and then putting the values in definition of harmonic index, we have

\[ HI(Z_s) = 5.9333333333n + 1I(Z_s, HI) = \log(HI) - \frac{1}{HI} \sum_{v \in V} \left( \frac{d_v}{d_v + d_v - 2} \right)^2 \log \left( \frac{d_v}{d_v + d_v - 2} \right) \]

\[ = \log(5.9333333333n + 1) - \frac{1}{5.9333333333n + 1} \left( 6(n + 4)(2)^n \log(2)^n + 4n(2)^n \log(2)^n + (4n - 3)(2.25)^n \log(2.25)^n \right) \]

**Theorem 7.** For Zig-Zag chain, the weighted entropy with harmonic index weight is

\[ I(Z_s, HI) = \log(5.9333333333n + 1) + 0.4916734472 + \frac{0.021057193}{n} + 2.175956732n. \]

**Proof.** Using the values in Table 1 and then putting the values in definition of harmonic index, we have

\[ HI(Z_s) = 5.9333333333n + 1I(Z_s, HI) = \log(HI) - \frac{1}{HI} \sum_{v \in V} \left( \frac{d_v}{d_v + d_v - 2} \right)^2 \log \left( \frac{d_v}{d_v + d_v - 2} \right) \]

\[ = \log(5.9333333333n + 1) - \frac{1}{5.9333333333n + 1} \left( 6(n + 4)(2)^n \log(2)^n + 4n(2)^n \log(2)^n + (4n - 3)(2.25)^n \log(2.25)^n \right) \]

**Theorem 8.** For Zig-Zag chain, the weighted entropy with sum-connectivity index weight is
Corollary 3.9. The weighted entropy for n=1 is

\[
I(Z_n, SCI) = \log(6.4218475439n + 0.7752551286) + 0.498852 + \frac{0.0195491428}{n} + 2.7610355373n.
\]

Proof. Using the values in Table 1 and then putting the values in definition of sum connectivity index, we have

\[
SCI(Z_n) = 6.4218475439n + 0.7752551286/I(Z_n, SCI)
\]

\[
= \log(SCI) - \frac{1}{SCI} \sum_{\text{edges}} \left( d_i + d_j \log \frac{1}{\sqrt{d_i + d_j}} \right)
\]

\[
= \log(6.4218475439n + 0.7752551286) - \frac{1}{6.4218475439n + 0.7752551286} \left( \frac{1}{\sqrt{6}}\log \frac{1}{\sqrt{6}} \right)
\]

\[
= \log(6.4218475439n + 0.7752551286) - \left( -0.9030899868n \right)
\]

\[
-0.6020599912 - 0.6553578353n + 0.4765183765n
= \log(6.4218475439n + 0.7752551286) - \left( -2.1636255999n \right)
\]

\[
-0.12554161148
= \log(6.4218475439n + 0.7752551286) - \left( -0.557184273n \right)
\]

\[
+ 1.2898979486n - 2.1636255999n - 0.12554161148
= \log(6.4218475439n + 0.7752551286) + 0.4988522471
\]

\[
+ 0.0195491428 + 2.790856228n.
\]

Conclusion

Weighted entropies of Zig-Zag chain of 8-cycles molecular graph was calculated by using probability density function by taking different topological indices as edge weight.

Acknowledgments

We are thankful to anonymous reviewers who have improved our paper.

Orcid:

Farkhanda Azfal:
https://orcid.org/0000-0001-5396-7598

Murat Cancan:
https://orcid.org/0000-0002-8606-2274

Mehmet Serif Aldemir:
https://orcid.org/0000-0002-5298-6743

References


**How to cite this article:** Farkhanda Afzal*, Sidra Razaq, Mehmoona Abdul Razaq, Murat Cancan, Mehmet Serif Aldemir. Weighted entropy of zig zag chain. *Eurasian Chemical Communications*, 2020, 2(10), 1082-1087.

Copyright © 2020 by SPC (Sami Publishing Company)+ is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.