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Weighted entropy of Zig-Zag chain

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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

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

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

Second Zagreb index $M_2(G)=\sum_{gh\in E(G)}(d_g.d_h)$

Atom-bond connectivity index

$$ABC(G)=\sum_{gh\in E(G)}\sqrt{\frac{d_g+d_h-2}{d_g.d_h}}$$

Augmented Zagreb index

$$AZI(G)=\sum_{gh\in E(G)}\left(\frac{d_g.d_h}{d_g+d_h-2}\right)^3$$

Geometric arithmetic index

$$GA(G)=\sum_{gh\in E(G)}\frac{2\sqrt{d_g.d_h}}{d_g+d_h}$$

Harmonic index $HI(G)=\sum_{gh\in E(G)}\frac{2}{d_g+d_h}$

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

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 $P_{ij}=\frac{w(uv)}{\sum W(uv)}$, then the entropy of graph G is defined as

$$I(G,w)=\sum P_{ij}\log P_{ij}.$$

Generalization of Zig-Zag chain graph

For $Z_8(n)$, for n≥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

$$I(Z_8(n),R)=\log(5.9663264952n+1)+0.4894192028+\frac{0.0209406468}{n}+2.174609452n.$$

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

$$R(Z_8(n))=5.9663264952n+1$$

$$I(Z_8,R)=\log(R)-\frac{1}{R}\sum_{gh\in E}\left(\frac{1}{\sqrt{d_g.d_h}}\log\frac{1}{\sqrt{d_g.d_h}}\right)$$

$$=\log(5.9663264952n+1)-\frac{1}{5.9663264952n+1}\Big((6n+4)\frac{1}{\sqrt{2.2}}\log\frac{1}{\sqrt{2.2}}+4n\frac{1}{\sqrt{2.3}}\log\frac{1}{\sqrt{2.3}}+(4n-3)\frac{1}{\sqrt{3.3}}\log\frac{1}{\sqrt{3.3}}\Big)$$

$$=\log(5.9663264952n+1)-\left(\frac{0.167607321}{n}+1\right)(-0.903089987n-0.6020599912-0.6353578352n-0.636161673n+0.4771212548)$$

$$=\log(5.9663265n+1)-\left(\frac{0.167607321}{n}+1\right)(-2.174609452n-0.1249387372)=\log(5.9663265n+1)-\left(-2.174609452n-0.1249387372-0.3644804656-\frac{0.0209406468}{n}\right)$$

$$=\log(5.9663264952n+1)+0.4894192028+\frac{0.0209406468}{n}+2.174609452n.$$

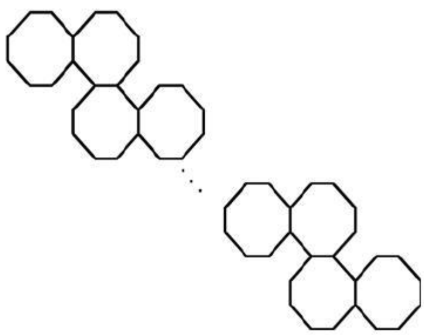

FIGURE 1. Zig-Zag Chain ($Z_8(n)$)

TABLE 1. Edge partition of of zig-zag chain

Edge	$(d_G(g);d_G(h))$	(2,2)	(2,3)	(3,3)
Vertices	frequencies	6n+4	4n	4n-3

Theorem 2. For Zig-Zag chain, the weighted Entropy with reciprocal Randić index is

$$I(Z_8(n), RR) = \log(33.7979589711n - 1) - 2.2749269537 + \frac{0.0557977874}{n} + 13.1499620172n.$$

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

$$RR(Z_8(n)) = 33.7979589711n - 1 I(Z_8, RR)) = \log(RR) - \frac{1}{RR}\sum_{gh\in E}(\sqrt{d_g.d_h}\log\sqrt{d_g.d_h})$$
$$= \log(33.7979589711n - 1) - \frac{1}{33.7979589711n - 1}(6n+4)\sqrt{2.2}\log\sqrt{2.2}$$
$$+4n\sqrt{2.3}\log\sqrt{2.3} + (4n-3)\sqrt{3.3})\log\sqrt{3.3}$$
$$= \log(33.7979589711n - 1) - (\frac{0.0295875855}{n} - 1) - (3.612359948n + 2.4082399653$$
$$+3.8121470123n + 5.7254550566n - 4.2940912925) = \log(33.7979589711n - 1)$$
$$-(\frac{0.0295875855}{n} - 1)(-1.8858513272 + 13.1499620172n) = \log(33.7979589711n - 1)$$
$$-(\frac{-0.0557977874}{n} + 0.3890756255 + 1.88588513272 - 13.1499620172n)$$
$$= \log(33.7979589711n - 1) - 2.2749269527 + \frac{0.0557977874}{n} + 13.1499620172n.$$

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

$$I(Z_8(n), M_1) = \log(68n - 2) + 2.8795941154 + \frac{0.0643200389}{n} + 23.5522349439n.$$
$$I(Z_8(n), M_2) = \log(84n - 11) - 2.2698151347 + \frac{0.192042713}{n} + 6.134354667n.$$

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

$$M_1(Z_8(n)) = 68n - 2 I(Z_8, M_1) = \log(M_1) - \frac{1}{M_1}\sum_{gh\in E}((d_g + d_h)\log(d_g + d_h))$$
$$= \log(68n - 2) - \frac{1}{68n - 2}((6n+4)(2+2)\log(2+2)$$
$$+4n(2+3)\log(2+3) + (4n-3)(3+3)\log(3+3))$$
$$= \log(68n - 2) - (\frac{0.0147058824}{n} - 0.5)(14.4494397919n + 9.6329598612$$
$$+13.9794000867n + 18.6756300092n - 14.00667225069)$$
$$= \log(68n - 2) - (\frac{0.0147058824}{n} - 0.5)(47.1044698878n - 4.3737626457)$$
$$= \log(68n - 2) - (0.6927127925 - \frac{0.0643200391}{n}$$
$$-23.5522349439n + 2.1868813229)$$
$$= \log(68n - 2) + 2.8795941154 + \frac{0.0643200389}{n} + 23.5522349439n.$$

$$M_2 = 84n - 11 I(Z_8, M_2) = \log(M_2) - \frac{1}{M_2}\sum_{gh\in E}((d_g.d_h)\log(d_g.d_h))$$
$$= \log(84n - 11) - \frac{1}{84n - 11}((6n+4)(2.2)\log(2.2)$$
$$+(4n)(2.3)\log(2.3) + (4n-3)(3.3)\log(3.3))$$
$$= \log(84n - 11) - (\frac{0.0119047619}{n} - 0.0909090909)$$
$$(14.4494397918n + 9.6329598612$$
$$+18.6756300092n + 34.3527303398n - 25.7645477549)$$
$$= \log(84n - 11)(\frac{0.0119047619}{n} - 0.0909090909)$$
$$(67.4778001408n - 16.1315878937)$$
$$= \log(84n - 11) - (0.8033071442 - \frac{0.1920427129}{n}$$
$$+1.4665079902 - 6.134354667n)$$
$$= \log(84n - 11) - 2.2698151347$$
$$+\frac{0.192042713}{n} + 6.134354667n.$$

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

$$I(Z_8, ABC) = \log(9.7377344785n + 0.8284271247) + 0.245667411 + \frac{0.0074991269}{n} + 1.8515552166n.$$

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

$$ABC(G) = 9.7377344785n + 0.8284271247 I(Z_8, ABC)$$
$$= \log(ABC) - \frac{1}{ABC}\sum_{gh\in E}(\sqrt{\frac{d_g + d_h - 2}{d_g.d_h}}\log\sqrt{\frac{d_g + d_h - 2}{d_g.d_h}})$$
$$= \log(9.7377344785n + 0.8284271247) - \frac{1}{9.737785n + 0.8284271247}$$
$$(6n+4)\sqrt{\frac{1}{2}}\log\sqrt{\frac{1}{2}} + (4n)\sqrt{\frac{1}{2}}\log\sqrt{\frac{1}{2}} + (4n-3)\frac{2}{3}\log\frac{2}{3}$$
$$= \log(9.7377344785n + 0.8284271247) - \Big(\frac{0.102693291}{n}$$
$$+1.207106813\Big)(-0.6385810538n - 0.4257207025 - 0.4257207024n$$
$$-0.46957676691n + 0.3521825181)$$
$$= \log(9.737734785n + 0.8284271247) - \Big(\frac{0.102693291}{n}$$
$$+1.207106813\Big)(-1.5338785229 - 0.0730245069)$$
$$= \log(9.7377344785n + 0.8284271247) - (-0.1575190335$$
$$-\frac{0.0074991269}{n} - 1.8515552166n - 0.0881483775)$$
$$= \log(9.7377344785n + 0.8284271247) + 0.245667411$$
$$+\frac{0.0074991269}{n} + 1.8515552166n.$$

Theorem 5. For Zig-Zag chain, the weighted entropy with augmented Zagreb index weight is

$$I(Z_8, AZI) = \log(125.5625n - 2.171875) + 55.4708179248 + \frac{0.0573844335}{n} - 3.3175626475n.$$

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

$$AZI(Z_8) = 125.5625n - 2.171875 I(Z_8, AZI)$$
$$= \log(AZI) - \frac{1}{AZI}\sum_{gh\in E}\left(\left(\frac{d_g.d_h}{d_g+d_h-2}\right)^3 \log\left(\frac{d_g.d_h}{d_g+d_h-2}\right)^3\right)$$
$$= \log(125.5625n - 2.171875) - \frac{1}{125.5625n - 2.171875}$$
$$((6n+4)(2)^3\log(2)^3 + 4n(2)^3\log(2)^3 + (4n-3)(2.25)^3\log(2.25)^3)$$

$$= \log(125.5625n - 2.171875) - \frac{1}{125.5625n - 2.171875}$$
$$(43.3483193754n + 28.8988795836 + 28.8988795836n$$
$$+48.1389479443n - 36.1042109583)$$
$$= \log(125.5625n - 2.171875) - (\frac{0.0079641613}{n}$$
$$-0.4604316547)(-7.2053313747 + 120.3861469034)$$
$$= \log(125.5625n - 2.171875) - (0.9587748969$$
$$-\frac{0.0573844335}{n} + 3.3175626475n - 54.4295928217)$$
$$= \log(125.5625n - 2.171875) + 55.4708179248$$
$$+\frac{0.0573844335}{n} - 3.3175626475n.$$

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

$$I(Z_8, GA) = \log(13.9191835885n + 1) + \frac{0.0024959184}{n}$$
$$+0.0347411464n. GA(Z_8) = 1 + 13.9191835885n$$

Proof. Using the values in Table 1 and then putting the values in definition geometric-arithmetic index, we have

$$I(Z_8, GA) = \log(GA) - \frac{1}{GA}\sum_{gh\in E}\left(\frac{2\sqrt{d_g.d_h}}{d_g+d_h}\log\frac{2\sqrt{d_g.d_h}}{d_g+d_h}\right)$$
$$= \log(13.9191835885n + 1) - \frac{1}{13.9191835885n + 1}$$
$$\left((6n+4)\frac{2\sqrt{2.2}}{2+2}\log\frac{2\sqrt{2.2}}{2+2} + (4n)\frac{2\sqrt{2.3}}{2+3}\log\frac{2\sqrt{2.3}}{2+3}\right.$$
$$\left.+(4n-3)\frac{2\sqrt{3.3}}{3+3}\log\frac{2\sqrt{3.3}}{3+3}\right)$$
$$= \log(13.9191835885n + 1) - \frac{1}{13.9191835885n + 1}(4n(-0.008652866))$$
$$= \log(13.9191835885n + 1) - \frac{1}{13.9191835885n + 1}(-0.0347411464n)$$
$$= \log(13.9191835885n + 1) - (\frac{0.0718432941}{n} + 1)(-0.0347411464n0)$$
$$= \log(13.9191835885n + 1) + \frac{0.0024959184}{n} + 0.0347411464n.$$

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

$$I(Z_8, HI) = \log(5.9333333333n + 1) + 0.4916734472$$
$$+\frac{0.021057193}{n} + 2.1759556732n.$$

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

$$HI(Z_8) = 5.9333333333n + 1 I(Z_8, HI) = \log(HI)$$
$$-\frac{1}{HI}\sum_{gh\in E}\frac{2}{d_g+d_h}\log\frac{2}{d_g+d_h}$$
$$= \log(5.9333333333n + 1) - \frac{1}{5.9333333333n + 1}$$
$$((6n+4)\frac{1}{2}\log\frac{1}{2} + (4n)\frac{2}{5}\log\frac{2}{5} + (4n-3)\frac{1}{3}\log\frac{1}{3})n$$
$$= \log(5.9333333333n + 1) - \frac{1}{5.9333333333n + 1}$$
$$(-0.9030899868n - 0.602060599912$$
$$-0.636704014n - 0.6361616732n + 0.4771212548)$$
$$= \log(5.9333333333n + 1) - \frac{1}{5.9333333333n + 1}$$
$$(-0.124939345 - 2.1759556732n)$$
$$= \log(5.9333333333n + 1) - (-0.3667341024$$
$$-\frac{0.0210570904}{n} - 0.1249387364 - 2.1759556732n)$$
$$= \log(5.9333333333n + 1) + 0.4917214664$$
$$\left(\frac{0.0210570904}{n}\right) + 2.1759556732n.$$

Theorem 8. For Zig-Zag chain, the weighted entropy with sum-connectivity index weight is

$$I(Z_8, SCI) = \log(6.4218475439n + 0.7752551286)$$
$$+0.498852 + \frac{0.0195491428}{n} + 2.7610355373n.$$

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

$$SCI(Z_8) = 6.4218475439n + 0.7752551286 I(Z_8, SCI)$$
$$= \log(SCI) - \frac{1}{SCI}\sum_{gh\in E}\left(\frac{1}{\sqrt{d_g+d_h}}\log\frac{1}{\sqrt{d_g+d_h}}\right)$$
$$= \log(6.4218475439n + 0.7752551286)$$
$$-\frac{1}{6.4218475439n + 0.7752551286}$$
$$\left((6n+4)\frac{1}{\sqrt{4}}\log\frac{1}{\sqrt{4}} + (4n)\frac{1}{\sqrt{5}}\log\frac{1}{\sqrt{5}} + (4n-3)\frac{1}{\sqrt{6}}\log\frac{1}{\sqrt{6}}\right)$$
$$= \log(6.4218475439n + 0.7752551286)$$
$$-\frac{1}{6.4218475439n + 0.7752551286}(-0.9030899868n$$
$$-0.6020599912 - 0.6251777776n$$
$$-0.6353578353n + 0.4765183765)$$
$$= \log(6.4218475439n + 0.7752551286)$$
$$-\frac{1}{6.4218475439n + 0.7752551286}(-2.1636255999n$$
$$-0.1255416148)$$
$$= \log(6.4218475439n + 0.7752551286) - \left(\frac{0.1557184273}{n}\right.$$
$$\left.+1.2898979486\right)(-2.1636255999n - 0.1255416148)$$
$$= \log(6.4218475439n + 0.7752551286) + 0.4988522471$$
$$+\frac{0.0195491428}{n} + 2.790856228n.$$

Corollary 3.9. The weighted entropy for n=1 is

$I(Z_8;R)=1.1730528649$;

$I(Z_8;RR)=1.1724074381$;

$I(Z_8;M_1)=1.1721089752$;

$I(Z_8;M_2)=1.1599500915$;

$I(Z_8;ABC)=1.1760459679$;

$I(Z_8;AZI)=1.1740259687$;

$I(Z_8;GA)=1.1743272138$;

$I(Z_8;HI)=1.1728018509$;

$I(Z_8;SCI)=1.1752255818$.

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.

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