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AMPLIFIED ECCENTRIC CONNECTIVITY INDEX OF GRAPHS

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Abstract. A new distance based graphical index, coined as amplified eccentric connectivity index, has been established and the formulae to calculate the amplified eccentric connectivity index of some standard graphs, Dutch windmill graph and molecular graph of cycloalkenes has been computed. Also, in the case of boiling points of primary and secondary amines, the study shows that the amplified eccentric connectivity index gives a greater correlation of 98%, when compared to the Wiener and Eccentric connectivity indices.

Keywords: Graphical index, Distance, Amplified eccentric connectivity index, Dutch windmill graph, Molecular graph, Cycloalkenes.

AMS Subject Classification: 05C07, 05C09, 05C12, 05C90, 05C92.

1. Introduction

Graphical indices play an important role in chemical graph theory, which deal with the classification and characterization of chemical structures. A fundamental concept of chemistry is that the structural characteristics of a molecule are responsible for its properties. Graphical indices are a convenient means of translating chemical constitution into numerical values which can be used for correlation with various physical properties, chemical reactivity or biological activity [1, 8]. These graph invariants are also called Topological indices as they characterize the topology of the molecular graphs [10]. The use of graphical indices in QSPR and QSAR studies has become a major interest in recent years [11]. Graphical indices have found applications in various areas of chemistry; namely, in chemical documentation, isomer discrimination and pharmaceutical drug design [9]. Some of the most widely known graphical indices are Winer index, Randić index, Reciprocal randić index, Zagreb index, Harmonic index, ABC index etc.

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Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. For a vertex $v \in V(G)$, the degree of v is denoted by $d(v)$ and is defined as the number of edges incident with v. For the vertices $u, v \in V(G)$, the distance between u and v is denoted by $d(u, v)$ and is defined as the length of the shortest path connecting u and v in G. The eccentricity of a vertex v is denoted by $e(v)$ and is maximum of $d(u, v)$ for all $u \in V(G)$ [3]. We consider simple, undirected, connected graph throughout this paper.

In 1997, the topological descriptor termed the eccentric connectivity index [7] is defined as

$$\xi^c(G) = \sum_{v \in V(G)} d(v)e(v),$$

which has numerous applications and studied extensively in [2, 5, 12]. Motivated by this and considering the enormous application of graphical indices to the study of physical, chemical and biological properties of chemical compounds, we have come up with a novel graphical index, entitled as amplified eccentric connectivity index and it is denoted by $\xi^{ac}(G)$.

Definition 1.1. *The amplified eccentric connectivity index of a graph G with at least one edge is defined as*

$$\xi^{ac}(G) = \sum_{uv \in E(G)} [d(u)e(u) + d(v)e(v)].$$

2. Main Results

We obtain the amplified eccentric connectivity index for some standard graphs.

Proposition 2.1. *For any complete graph K_n, $\xi^{ac}(K_n) = n(n-1)^2$.*

Proof. In K_n, $d(v) = n - 1$ and $e(v) = 1$, $\forall\ v \in V(K_n)$.

$$\begin{aligned}\xi^{ac}(K_n) =& \sum_{uv \in E(K_n)} [d(u)e(u) + d(v)e(v)]\\ =&[(n-1)(1) + (n-1)(1)] + ... + [(n-1)(1) + (n-1)(1)]\\ =&n(n-1)^2.\end{aligned}$$

□

Proposition 2.2. *For any wheel graph W_n $(n \geq 5)$, $\xi^{ac}(W_n) = (n-1)(n+17)$.*

Proof. Let v_0 be the central vertex of W_n. Then, $d(v_0) = n - 1$, $e(v_0) = 1$ and $d(v_i) = 3$, $e(v_i) = 2$ where, $i = 1, 2, 3, ..., n - 1$.
Therefore,

$$\begin{aligned}\xi^{ac}(W_n) =&[(n-1)(1) + (3)(2)] + ... + [(n-1)(1) + (3)(2)]\\ &+ [(3)(2) + (3)(2)] + ... + [(3)(2) + (3)(2)]\\ =&(n-1)(n+17).\end{aligned}$$

□

Proposition 2.3. *For any complete bipartite graph $K_{m,n}$ $(m, n \geq 2)$,*

$$\xi^{ac}(K_{m,n}) = 2mn(m+n).$$

Proof. In $K_{m,n}$, we have $d(u_i) = n$, $e(u_i) = 2$ where, $i = 1, 2, 3, ..., m$ and $d(v_j) = m$, $e(v_j) = 2$ where, $j = 1, 2, 3, ..., n$. Then,

$$\begin{aligned}\xi^{ac}(K_{m,n}) =&[(n)(2) + (m)(2)] + ... + [(n)(2) + (m)(2)]\\ &+[(n)(2) + (m)(2)] + ... + [(n)(2) + (m)(2)]\\ &\vdots\\ &+[(n)(2) + (m)(2)] + ... + [(n)(2) + (m)(2)]\\ =&2mn(m + n).\end{aligned}$$

□

Proposition 2.4. *For any star $K_{1,n}$ $(n \geq 2)$, $\xi^{ac}(K_{1,n}) = n(n + 2)$.*

Proof. Let v_0 be the central vertex of the star graph $K_{1,n}$. Then, $d(v_0) = n$, $e(v_0) = 1$ and $d(v_i) = 1$, $e(v_i) = 2$ where, $i = 1, 2, 3, ..., n$.

By the definition of ξ^{ac}, we have,

$$\begin{aligned}\xi^{ac}(K_{1,n}) =&[(n)(1) + (1)(2)] + ... + [(n)(1) + (1)(2)]\\ =&n(n + 2).\end{aligned}$$

□

Proposition 2.5. *For any cycle C_n $(n \geq 3)$,*

$$\xi^{ac}(C_n) = \begin{cases} 2n^2, & \text{if } n \text{ is even;} \\ 2n^2 - 2n, & \text{if } n \text{ is odd.} \end{cases}$$

Proof. In C_n, $d(v_i) = 2$, $i = 1, 2, 3, ..., n$. We consider the following cases.

Case(i): If n is even, then $e(v_i) = \frac{n}{2}$, $i = 1, 2, 3, ..., n$. We have

$$\begin{aligned}\xi^{ac}(C_n) =& \left[(2)\left(\frac{n}{2}\right) + (2)\left(\frac{n}{2}\right)\right] + ... + \left[(2)\left(\frac{n}{2}\right) + (2)\left(\frac{n}{2}\right)\right]\\ =&2n^2.\end{aligned}$$

Case(ii): If n is odd, then $e(v_i) = \frac{n-1}{2}$, $i = 1, 2, 3, ..., n$. We have

$$\begin{aligned}\xi^{ac}(C_n) =& \left[(2)\left(\frac{n-1}{2}\right) + (2)\left(\frac{n-1}{2}\right)\right] + ... + \left[(2)\left(\frac{n-1}{2}\right) + (2)\left(\frac{n-1}{2}\right)\right]\\ =&2n^2 - 2n.\end{aligned}$$

□

Proposition 2.6. *For any path P_n,*

$$\xi^{ac}(P_n) = \begin{cases} 3n^2 - 8n + 6, & \text{if } n \text{ is even;} \\ 3n^2 - 8n + 5, & \text{if } n \text{ is odd.} \end{cases}$$

Proof. In a path P_n with $V(P_n) = \{v_1, v_2, v_3, ..., v_n\}$, we have $d(v_1) = d(v_n) = 1$ and $d(v_i) = 2$, $2 \leq i \leq n - 1$. We consider the following cases.

Case(i): If n is even, then $e(v_1) = e(v_n) = n - 1$, $e(v_2) = e(v_{n-1}) = n - 2$, ..., $e\left(v_{\frac{n}{2}}\right) = e\left(v_{\frac{n}{2}+1}\right) = \frac{n}{2}$. We have

$$\begin{aligned}\xi^{ac}(P_n) =&[(1)(n-1)+(2)(n-2)]+[(2)(n-2)+(2)(n-3)]\\&+...+\left[(2)\left(\frac{n}{2}\right)+(2)\left(\frac{n}{2}\right)\right]+...\\&+[(2)(n-3)+(2)(n-2)]+[(2)(n-2)+(1)(n-1)]\\=&3n^2-8n+6.\end{aligned}$$

Case(ii): If n is odd, then $e(v_1) = e(v_n) = n-1$, $e(v_2) = e(v_{n-1}) = n-2$, ..., $e\left(v_{\frac{n+1}{2}-1}\right) = e\left(v_{\frac{n+1}{2}+1}\right) = \frac{n-3}{2}$ and $e\left(v_{\frac{n+1}{2}}\right) = \frac{n-1}{2}$. We have

$$\begin{aligned}\xi^{ac}(P_n) =&[(1)(n-1)+(2)(n-2)]+[(2)(n-2)+(2)(n-3)]+...\\&+\left[(2)\left(\frac{n-3}{2}\right)+(2)\left(\frac{n-1}{2}\right)\right]+\left[(2)\left(\frac{n-1}{2}\right)+(2)\left(\frac{n-3}{2}\right)\right]+...\\&+[(2)(n-3)+(2)(n-2)]+[(2)(n-2)+(1)(n-1)]\\=&3n^2-8n+5.\end{aligned}$$ □

In order to test the validity of the conceived graphical index, we examine the relationship of amplified eccentric connectivity index with boiling points of primary and secondary amines. For this, we consider the hydrogen-suppressed molecular graph of each amines and calculate the value of ξ^{ac}. We take the experimental values of the boiling point of a group of 21 primary and 13 secondary amines from [7]. By subjecting these datasets to non-linear regression analysis, we get the corresponding fitting equations along with their correlation coefficients, average error (calculated from the percentage error of each amine), and root mean square (RMS) errors as displayed in the Tables 2.1 and 2.2.

		Boiling points ℃					Boiling points ℃		
			predicted					predicted	
Compound	ξ^{ac}	exptl	a	b	Compound	ξ^{ac}	exptl	a	b
				Primary Amines					
n-propylamine	22	49	49.23	44.74	4-methylpentylamine	91	125	124.07	117.03
2-aminopropane	15	33	39.48	35.02	n-hexylamine	96	130	128.19	120.86
2-amino-2-methylpropane	20	46	46.49	42.02	3-methylpentylamine	83	114	117.15	110.54
2-aminobutane	35	63	66.19	61.50	4-aminoheptane	115	139	142.54	134.10
2-methylpropylamine	35	69	66.19	61.50	2-aminoheptane	127	142	150.63	141.46
n-butylamine	40	77	72.32	67.51	n-heptylamine	134	155	155.03	145.45
2-amino-2-methylbutane	52	78	86.23	81.04	n-octylamine	176	180	177.37	165.65
2-aminopentane	59	92	93.81	88.35	n-nonylamine	226	201	198.02	185.33
3-methylbutylamine	59	96	93.81	88.35	2-aminoundecane	323	237	237.83	233.28
2-methylbutylamine	50	96	83.99	78.87	3-aminopentane	53	91	87.34	82.11
n-pentylamine	66	104	101.04	94.28					
				Secondary Amines					
N-(methyl)ethylamine	22	36	35.69	44.74	N-methyl-1-methylbutylamine	85	105	100.52	112.20
N-methyl-1-methylethylamine	35	50	51.92	61.49	dipropylamine	96	109.5	108.77	120.86
diethylamine	40	56	57.72	67.51	bis(2-methylpropyl)amine	158	139	144.21	157.66
N-methyl-1-methylpropylamine	53	78.5	71.76	82.11	dibutylamine	176	159	152.28	165.65
N-(ethyl)propylamine	66	80.5	84.38	95.28	bis(3-methylbutyl)amine	262	187.5	191.65	199.99
bis(1-methylethyl)amine	78	84	94.87	106.27	dipentylamine	280	205	202.32	208.34
N-(methyl)butylamine	66	90.5	84.38	95.28					

Here 'a' represents the predicted value of each compound for primary and secondary amines as different datasets and 'b' represents the predicted value of each compound for the combined datasets.

Table 2.1: Relationship of Amplified eccentric connectivity index (ξ^{ac}) with Boiling Points of Primary and Secondary Amines.

Boiling point	n	Equations	cc (%)	av (%)	RMS (%)
Of primary amines	21	bp = 17.04 + 1.569 ξ^{ac} - $4.93\times10^{-3}(\xi^{ac})^2$ + $6.779\times10^{-6}(\xi^{ac})^3$	99.60	4.16	6.26
Of secondary amines	13	bp = 4.228 + 1.553 ξ^{ac} - $5.775\times10^{-3}(\xi^{ac})^2$ + $9.845\times10^{-6}(\xi^{ac})^3$	99.48	4.40	5.49
Of both primary and secondary amines	34	bp = 12.46 + 1.586 ξ^{ac} - $5.589\times10^{-3}(\xi^{ac})^2$ + $8.654\times10^{-6}(\xi^{ac})^3$	98.11	9.13	11.31

Here 'bp' represents boiling point, 'cc' stands for correlation coefficient, 'av' for average error, 'RMS' for root mean square error and 'n' is the number of amines taken into consideration.

Table 2.2: Correlation of Amplified eccentric connectivity index (ξ^{ac}) with Boiling Points of Primary and Secondary Amines.

From the Table 2.2, it is noticeable that the amplified eccentric connectivity index has a striking correlating ability due to its minimal average and RMS errors. Comparing these correlations with that of the Eccentric connectivity and Weiner indices whose correlation coefficients are 97% and 92% respectively, as computed in [7], we find that amplified eccentric connectivity index has the better predicting ability in the case of boiling points of both primary and secondary amines.

3. Cycloalkenes

Cycloalkenes are used for biological and industrial purposes in the production of molecules essential to a broad spectrum of applications. We consider a cycloalkene having n carbon atoms and $2n-2$ hydrogen atoms and denoted by C_n^{2n-2}. The molecular graph of cycloalkenes is obtained by attaching $2n-2$ pendant vertices corresponding to hydrogen atoms to vertices of a cycle corresponding to carbon atoms as shown in Figure 3.1 [6]. We calculate the amplified eccentric connectivity index of this molecular graph.

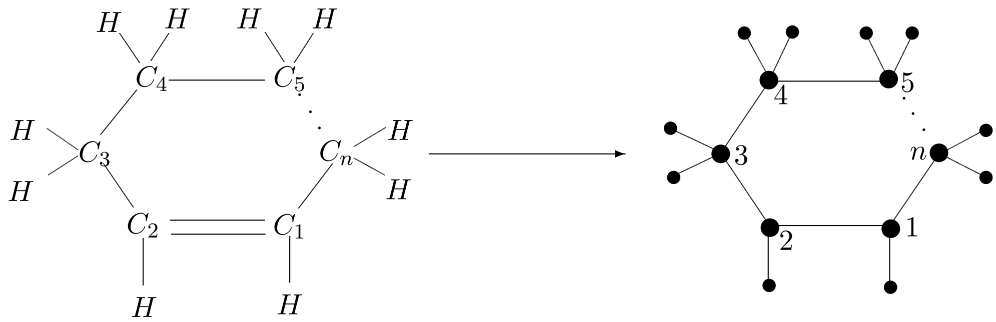

Figure 3.1 A cycloalkene and it's molecular graph

Theorem 3.1. *Let $n \geq 3$ be a positive integer. Then the amplified eccentric connectivity index of the graph C_n^{2n-2} is*

$$\xi^{ac}(C_n^{2n-2}) = \begin{cases} 9n^2 + 12n - 18, & \text{if } n \text{ is even;} \\ 9n^2 + 3n - 10, & \text{if } n \text{ is odd.} \end{cases}$$

Proof. Consider the molecular graph C_n^{2n-2} of a cycloalkene. This graph has $3n-2$ vertices. Two of these vertices corresponding to carbon atoms of cycloalkenes are of degree 3, and

$n-2$ vertices corresponding to carbon atoms are of degree 4. The remaining $2n-2$ vertices correspond to hydrogen atoms of cycloalkenes and they are pendant vertices. We have the following cases.

Case (i): If n is even then, the eccentricity of each vertex corresponding to carbon atom is $\frac{n}{2}+1$. The eccentricity of each vertex corresponding to hydrogen atoms is $\frac{n}{2}+2$. So we have

$$\begin{aligned}
\xi^{ac}(C_n^{2n-2}) = &\sum_{uv\in E(C_n^{2n-2})} [d(u)e(u)+d(v)e(v)] \\
=&(n-3)\left[4\left(\frac{n}{2}+1\right)+4\left(\frac{n}{2}+1\right)\right] \\
&+2\left[4\left(\frac{n}{2}+1\right)+3\left(\frac{n}{2}+1\right)\right] \\
&+1\left[3\left(\frac{n}{2}+1\right)+3\left(\frac{n}{2}+1\right)\right] \\
&+(2n-4)\left[4\left(\frac{n}{2}+1\right)+1\left(\frac{n}{2}+2\right)\right] \\
&+2\left[3\left(\frac{n}{2}+1\right)+1\left(\frac{n}{2}+2\right)\right] \\
=&9n^2+12n-18.
\end{aligned}$$

Case (ii): If n is odd then, the eccentricity of each vertex corresponding to carbon atom is $\frac{n-1}{2}+1$. The eccentricity of each vertex corresponding to hydrogen atoms is $\frac{n-1}{2}+2$. So we have

$$\begin{aligned}
\xi^{ac}(C_n^{2n-2}) =&(n-3)\left[4\left(\frac{n-1}{2}+1\right)+4\left(\frac{n-1}{2}+1\right)\right] \\
&+2\left[4\left(\frac{n-1}{2}+1\right)+3\left(\frac{n-1}{2}+1\right)\right] \\
&+1\left[3\left(\frac{n-1}{2}+1\right)+3\left(\frac{n-1}{2}+1\right)\right] \\
&+(2n-4)\left[4\left(\frac{n-1}{2}+1\right)+1\left(\frac{n-1}{2}+2\right)\right] \\
&+2\left[3\left(\frac{n-1}{2}+1\right)+1\left(\frac{n-1}{2}+2\right)\right] \\
=&9n^2+3n-10.
\end{aligned}$$

□

4. Chemical compound $C_n^{R_r}$

$C_n^{R_r}$ is constructed by attaching alkyl R_r instead of each hydrogen atom in the cycloalkenes [6]. The molecular structure of $C_n^{R_r}$ is as shown in the Figure 4.1. In this section, we establish a general formula for the amplified eccentric connectivity index for the molecular graph $C_n^{R_r}$.

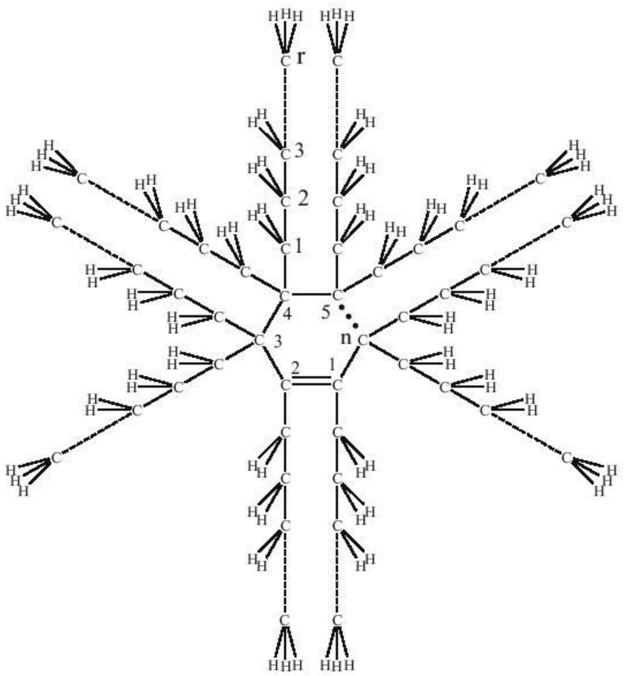

Figure 4.1 Molecular structure of $C_n^{R_r}$

Theorem 4.1. *Let n and r be positive integers with $n \geq 3$. Then the amplified eccentric connectivity index of a graph $C_n^{R_r}$ is*

$$\xi^{ac}(C_n^{R_r}) = \begin{cases} (18r+9)n^2 + (54r^2+60r+12)n - (54r^2+76r+18), & \text{if } n \text{ is even;} \\ \\ (18r+9)n^2 + (54r^2+42r+3)n - (54r^2+58r+10), & \text{if } n \text{ is odd.} \end{cases}$$

Proof. Consider the graph $G = C_n^{R_r}$ with $|V(G)| = 6nr + 3n - 6r - 2$. It has $n + 2nr - 2r$ vertices corresponding to the carbon atoms of $C_n^{R_r}$, n of them represent vertices of the cycle, out of which two have degree 3 and the remaining $n-2$ have degree 4. The other $2nr - 2r$ vertices not on the cycle of $C_n^{R_r}$ have the same degree 4. G also has $4nr+2n-4r-2$ pendant vertices corresponding to the hydrogen atoms of $C_n^{R_r}$. The eccentricities of the vertices of $C_n^{R_r}$ are shown in the Table 4.1.

Vertex corresponding to	Number of vertices	Eccentricity	
		for even n	for odd n
carbon atom on cycle	n	$\frac{n}{2}+r+1$	$\frac{n-1}{2}+r+1$
carbon atom not on cycle	$2nr-2r$	$\frac{n}{2}+r+1+i$, $1 \leq i \leq r$	$\frac{n-1}{2}+r+1+i$, $1 \leq i \leq r$
hydrogen atom	$4nr+2n-4r-2$	$\frac{n}{2}+r+i+2$, $1 \leq i \leq r$	$\frac{n-1}{2}+r+i+2$, $1 \leq i \leq r$

Table 4.1: Eccentricities of vertices of $C_n^{R_r}$

Case (i): If n is even, then

$$\begin{aligned}
\xi^{ac}(C_n^{R_r}) = &\sum_{uv\in E(C_n^{R_r})} [d(u)e(u)+d(v)e(v)]\\
=&(n-3)\left[4\left(\frac{n}{2}+r+1\right)+4\left(\frac{n}{2}+r+1\right)\right]\\
&+2\left[4\left(\frac{n}{2}+r+1\right)+3\left(\frac{n}{2}+r+1\right)\right]\\
&+1\left[3\left(\frac{n}{2}+r+1\right)+3\left(\frac{n}{2}+r+1\right)\right]\\
&+(2n-4)\left[4\left(\frac{n}{2}+r+1\right)+4\left(\frac{n}{2}+r+2\right)\right]\\
&+2\left[3\left(\frac{n}{2}+r+1\right)+4\left(\frac{n}{2}+r+2\right)\right]\\
&+(2n-2)\sum_{i=1}^{r-1}\left[4\left(\frac{n}{2}+r+1+i\right)+4\left(\frac{n}{2}+r+2+i\right)\right]\\
&+2(2n-2)\sum_{i=1}^{r}\left[4\left(\frac{n}{2}+r+1+i\right)+1\left(\frac{n}{2}+r+2+i\right)\right]\\
&+(2n-2)\left[4\left(\frac{n}{2}+2r+1\right)+1\left(\frac{n}{2}+2r+2\right)\right]\\
=&(18r+9)n^2+(54r^2+60r+12)n-(54r^2+76r+18).
\end{aligned}$$

Case (ii): If n is odd, then

$$\begin{aligned}
\xi^{ac}(C_n^{R_r}) =&(n-3)\left[4\left(\frac{n-1}{2}+r+1\right)+4\left(\frac{n-1}{2}+r+1\right)\right]\\
&+2\left[4\left(\frac{n-1}{2}+r+1\right)+3\left(\frac{n-1}{2}+r+1\right)\right]\\
&+1\left[3\left(\frac{n-1}{2}+r+1\right)+3\left(\frac{n-1}{2}+r+1\right)\right]\\
&+(2n-4)\left[4\left(\frac{n-1}{2}+r+1\right)+4\left(\frac{n-1}{2}+r+2\right)\right]\\
&+2\left[3\left(\frac{n-1}{2}+r+1\right)+4\left(\frac{n-1}{2}+r+2\right)\right]\\
&+(2n-2)\sum_{i=1}^{r-1}\left[4\left(\frac{n-1}{2}+r+1+i\right)+4\left(\frac{n-1}{2}+r+2+i\right)\right]\\
&+2(2n-2)\sum_{i=1}^{r}\left[4\left(\frac{n-1}{2}+r+1+i\right)+1\left(\frac{n-1}{2}+r+2+i\right)\right]\\
&+(2n-2)\left[4\left(\frac{n-1}{2}+2r+1\right)+1\left(\frac{n-1}{2}+2r+2\right)\right]\\
=&(18r+9)n^2+(54r^2+42r+3)n-(54r^2+58r+10).
\end{aligned}$$

$\square$

5. Dutch Windmill graph D_m^n

Dutch windmill graph [4] D_m^n is a graph obtained by joining n copies of cycle C_m with a common central vertex v_0, as shown in the Figure 5.1. In this section, we compute the amplified eccentric connectivity index of D_m^n.

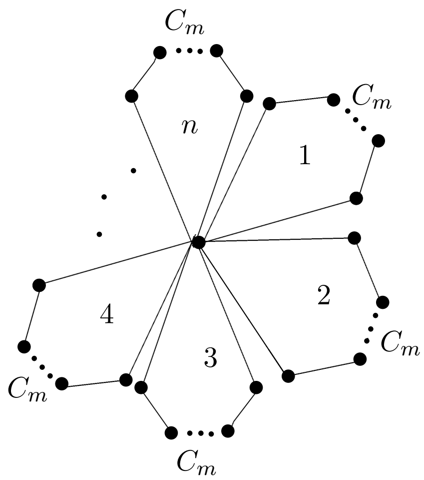

Figure 5.1 Dutch Windmill graph D_m^n

Theorem 5.1. *Let n and m be positive integers with $m \geq 3$. Then the amplified eccentric connectivity index of D_m^n is*

$$\xi^{ac}(D_m^n) = \begin{cases} (2m)n^2 + (3m^2 - 2m)n, & \text{if } n \text{ is even;} \\ \\ (2m-2)n^2 + (3m^2 - 4m + 1)n, & \text{if } n \text{ is odd.} \end{cases}$$

Proof. Consider the graph $G = D_m^n$ with vertices $(m-1)n+1$ having common central vertex v_0 of degree, $d(v_0) = 2n$ and $d(u) = 2$, $\forall\, u \in V(D_m^n)$. We have the following cases.

Case (i): If m is even, then each cycle of D_m^n has an odd number of vertices excluding the central vertex. Among these, each pair of vertices which are equidistant from the central vertex have the same eccentricity.

The eccentricity of central vertex $e(v_0) = \frac{m}{2}$ and for other vertex pair, it increases by one as we move away from the central vertex. The eccentricities of the vertices of D_m^n are shown in the Table 5.1.

Type of vertices	No. of vertices	Eccentricity	Degree
central vertex(v_0)	1	$\frac{m}{2}$	$2n$
vertices on each cycle other than both central vertex and a vertex at a distance $\frac{m}{2}$ from the central vertex	$(m-2)n$	$\frac{m}{2}+i$, $1 \leq i \leq \frac{m}{2}-1$	2
vertex on each cycle at a distance $\frac{m}{2}$ from the central vertex	n	m	2

Table 5.1: Eccentricities of vertices of D_m^n for even m.

The amplified eccentric connectivity index of D_m^n is

$$\begin{aligned}\xi^{ac}(D_m^n) &= \sum_{uv\in E(D_m^n)} [d(u)e(u)+d(v)e(v)]\\ &=(2n)\left[2n\left(\frac{m}{2}\right)+2\left(\frac{m}{2}+1\right)\right]\\ &\quad+(2n)\sum_{i=1}^{\frac{m}{2}-1}\left[2\left(\frac{m}{2}+i\right)+2\left(\frac{m}{2}+i+1\right)\right]\\ &=(2m)n^2+(3m^2-2m)n.\end{aligned}$$

Case (ii): If m is odd, then the eccentricity of the central vertex is $e(v_0)=\frac{m-1}{2}$ and eccentricity of other vertices increase by one as we move away from the common vertex of the half of the cycle.

When m is odd, the vertices other than the common vertex are even in number in each cycle. The Table 5.2 shows the corresponding eccentricity and degree of the vertices, in each cycle which are pairwise equal.

Types of vertices	No. of vertices	Eccentricity	Degree
central vertex(v_0)	1	$\frac{m-1}{2}$	$2n$
vertices on each cycle other than both central vertex and two vertices at a distance $\frac{m-1}{2}$ from the central vertex	$(m-1)n$	$\frac{m-1}{2}+i$, $1\le i\le \frac{m-1}{2}-1$	2
Two vertices on each cycle at a distance $\frac{m-1}{2}$ from the central vertex	n	$m-1$	2

Table 5.2: Eccentricities of vertices of D_m^n for odd m.

Therefore,

$$\begin{aligned}\xi^{ac}(D_m^n) &=(2n)\left[2n\left(\frac{m-1}{2}\right)+2\left(\frac{m-1}{2}+1\right)\right]\\ &\quad+(2n)\sum_{i=1}^{\frac{m-1}{2}-1}\left[2\left(\frac{m-1}{2}+i\right)+2\left(\frac{m-1}{2}+i+1\right)\right]\\ &\quad+(n)[2(m-1)+2(m-1)]\\ &=(2m-2)n^2+(3m^2-4m+1)n.\end{aligned}$$ □

6. Conclusions

In this paper, we have proposed a new distance based graphical index named, amplified eccentric connectivity index, which is found out to be a better predictor in the case of boiling point of amines with more than 98% of correlation coefficient. Further, we have formulated the amplified eccentric connectivity index of some standard graphs and few chemical structures, by means of graph theory and mathematical derivations.

References

[1] Babujee, J. B. and Ramakrishnan, S., (2012), Topological Indices and New Graph Structures, Appl. Math. Sci., 108, (6), pp. 5383-5401.
[2] Bantva, D., (2018), On a lower bound for the eccentric connectivity index of graphs, Discret. Appl. Math., 10743, pp. 179-187.
[3] Harary, F., (1969), Graph Theory, Addison Wesley, Reading Mass.
[4] Idrees, N., Saif, M. J. and Anwar, T., (2019), Eccentricity-Based Topological Invariants of Some Chemical Graphs, Atoms, 7, (1), Article 21.
[5] Ilić, A., (2010), Eccentric connectivity index, Novel Molecular Structure Descriptors-Theory and Applications II, 9, pp. 139-168.
[6] Mathad, V., Padmapriya, P. and Cangul, I. N., (2019), Some topological indices of certain classes of cycloalkenes, Proc. Jangjeon Math. Soc., 22, (2), pp. 233-247.
[7] Sharma, V., Goswami, R. and Madan, A. K., (1997), Eccentric Connectivity Index: A Novel Highly Discriminating Topological Descriptor for Structure-Property and Structure-Activity Studies, J. Chem. Inf. Comput. Sci., 37, pp. 273-282.
[8] Shirakol, S., Kalyanshetti, M. and Hosamani S. M., (2019), QSPR Analysis of certain Distance Based Topological Indices, Applied Mathematics and Nonlinear Sciences, 4, (2), pp. 371-386.
[9] Tang, L., Wang, X., Liu, W. and Feng, L., (2017), The extremal values of connective eccentricity index for trees and unicyclic graphs, Int. J. Comput Math., 94, (3), pp. 437-453.
[10] Trinajstić, N., (1983), Chemical graph theory, CRC Press, Boca Raton.
[11] Yan, L., Farahani, M. R. and Gao, W., (2018), Distance-based Indices Computation of Symmetry Molecular Structures, Open Journal of Mathematical Sciences, 2, (1), pp. 323-337.
[12] Zhou, B. and Du, Z., (2010), On eccentric connectivity index, Match-Commun. Math. Co., 63, (1), pp. 181-198.

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