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Eccentricity based indices for some classes Fence graphs

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Abstract. One of the most important ideas employed in chemical graph theory is that of so-called topological indices. This is to associate a numerical value with a graph structure that often has some kind of correlation with corresponding chemicals properties. In this paper, we consider some infinite families of 3-fence graphs, namely, ladder, circular ladder and Mobius ladder. We compute some of the eccentricity based topological indices of these graphs and their line graphs.

Keywords. eccentricity, topological index, 3-fence graphs.

1 Introduction

All graphs considered in this paper are simple and connected. Let $N_G(v)$ be the set of all neighbors of a vertex v in a graph G. The degree $d_G(v)$ of a vertex v in G is the cardinality of the set $N_G(v)$. A vertex with degree one is called a pendent vertex. *The eccentricity* of a vertex v, denoted by $\epsilon_G(u)$, is the largest distance from v to any other vertex u of G. The line graph $\Gamma(G)$ of a graph G is a graph with vertex set $V(\Gamma(G)) = E(G)$ and two vertices in $\Gamma(G)$ are adjacent if the corresponding edges in G have a common end-vertex.

Chemical graph theory is the topological branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena. Quantitative structure- activity relationship models (QSAR models) are regression or classification models used in the chemical and biological sciences and control system engineering. One of the first historical QSAR chemical applications was to predict boiling points. *A topological indices* of molecular chemical graphs is a numerical value associated with chemical constitution for correlation of chemical structure with various Physical properties, chemical reactivity or biological activity. Topological indices are the useful tools provided by graph theory for theoretical study of chemical compounds and it plays an important role in studying certain

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topological properties of chemical compounds especially organic materials, that is, carbon containing molecular structures. Hundreds of papers have been published in the field of topological indices of these nanostructures to study their topologies using mathematical or more precisely graph- theoretic tools. Molecules and molecular compounds are often modeled by molecular graph. A molecular graph is a representation of the structural formula for chemical compound whose vertices correspond to the atoms of the compound and edge correspond to chemical bounds.

In recent years, Some indices have been derived related to eccentricity such as eccentric connectivity index, eccentric distance sum, adjacent distance sum, total eccentricity index. The eccentric connectivity index was successfully used for mathematical models of biological activities of diverse nature [3, 4, 6]. It has been shown to give a high degree of predictability of pharmaceutical properties, and provide leads for the development of safe and potent anti-HIV compounds [7]. Eccentric connectivity index is also proposed as a measure of branching in alkanes [8].

In this sequence, Malik [9] proposed variant of topological descriptors related to eccentricity, namely, the inverse connective eccentricity index and inverse total eccentricity index which are defined for a connected graph G as $\xi_{ce}^{-1}(G) = \sum\limits_{u \in V(G)} \frac{\epsilon_G(u)}{d_G(u)}$ $\zeta^{-1}(G) = \sum\limits_{u \in V(G)} \frac{1}{\epsilon_G(u)}$.

The eccentric connectivity polynomial is the polynomial version of the eccentric-connectivity index which was proposed by Alaeiyan et.al. [5] and it is defined for a connected graph G as $ECP(G,x) = \sum\limits_{u \in V(G)} d_G(u) x^{\epsilon_G(u)}$. The inverse degree index denoted by $ID(G)$ of a graph G is defined as $ID(G) = \sum\limits_{u \in V(G)} \frac{1}{d_G(u)}$. The inverse degree (also known as the sum of reciprocals of degrees) first attracted attention through numerous conjectures generated by the computer programme by Graffiti [2].

In this paper, we study on some of the eccentricity based topological indices for infinite families of 3-fence graphs such as ladder, circular ladder and Mobius ladder and their line graphs.

2 Some 3- Fence graphs and their eccentric- connectivity indices

$L[n]$ denotes ladder graph with n cycles of length 4 is shown in Figure 1. The number of vertices and edges of $L[n]$ are $2n+2$ and $3n+1$, respectively. We define the circular ladder with $n \geq 2$ is denoted by $CL[n]$ which is obtained from the ladder graph $L[n]$ by joining the vertices u_n with u_1 and v_n with v_1. The number of vertices and edges of $CL[n]$ are respectively, given $2n+2$ and $3n+3$. On twisting a single time. In a circular ladder graph $CL[n]$ is graph called Mobius ladder or Mobius strip and it is represented by $ML[n]$. The number of vertices and edges are same both in $CL[n]$ and $ML[n]$. The following Table shows the various eccentricity of $L[n]$ with respect to the its vertex partition.

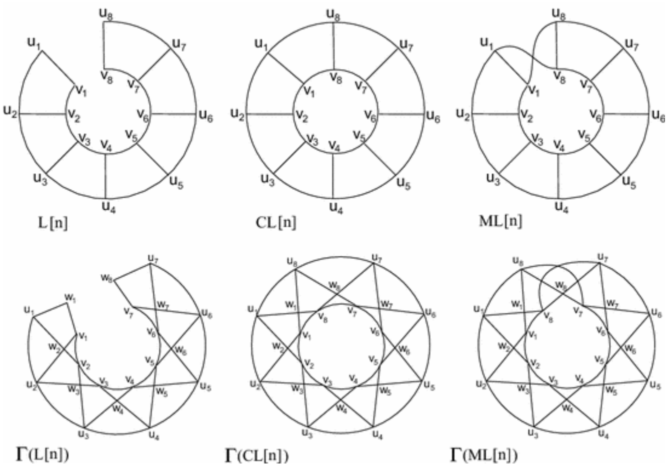

Figure 1.

Table 1. The ladder graph $L[n]$with n cycle.

Vertices	Degree	Eccentricity	Frequency
u_1	2	$n+1$	4
$u_i(2 \leq i \leq \lceil \frac{n}{2} \rceil)$, n is odd	3	$n-i+2$	4
$u_i(2 \leq i < \frac{n+2}{2})$, n is odd	3	$n-i+2$	4
$u_{\frac{n+2}{2}}$	3	$\frac{n+2}{2}$	2

Theorem 2.1. Let n be a positive integer. Then the inverse connective eccentricity index of $G = L[n]$ is

$$\xi_{ce}^{-1}(G) = \begin{cases} \frac{2}{3}(2(nr + r^2 + 3r) + n - 5) & \text{if } n \text{ is odd,} \\ \frac{1}{3}(4nr - 2r^2 + 4) + n + 2r & \text{if } n \text{ is even.} \end{cases}$$

Proof: By the proof is given for of n, that is, odd and even. By the definition inverse connective eccentricity,

$$\xi_{ce}^{-1}(G) = \sum_{u \in V(G)} \frac{\epsilon_G(u)}{d_G(u)}.$$

By Table 1, and if n is odd, we have

$$\begin{aligned} \xi_{ce}^{-1}(G) &= 2(n+1) + \sum_{i=2}^{r} \frac{4(n+2-i)}{3} \\ &= 2(n+1) + \frac{(n+2)(4r-3)}{3} - \frac{4(r^2+r-2)}{6} \\ &= \frac{2}{3}(2(nr + r^2 + 3r) + n - 5). \end{aligned}$$

By Table 1 and if n is even, we have

$$\begin{aligned}\xi_{ce}^{-1}(G) &= 2(n+1) + \frac{n+2}{3} + \sum_{i=2}^{r} \frac{4(n+2-i)}{3} \\ &= 2(n+1) + \frac{(n+2)(4r-3)}{3} - \frac{4(r^2+r-2)}{6} \\ &= \frac{1}{3}(4nr - 2r^2 + 4) + n + 2r.\end{aligned}$$

Corollary 2.2. Let n be a positive integer. Then $G = L[n]$ is

$$(i)\ \ ECP(G,x) = \begin{cases} 2x^{4(n+1)} + 3x^{4nr-2r^2-10r-4n-4} & \text{if } n \text{ is odd,} \\ 2x^{4(n+1)} + 3x^{4nr-2r^2+10r-3n-2} & \text{if } n \text{ is even.} \end{cases}$$

$$(ii)\ \ \zeta^{-1}(G) \leq \begin{cases} \frac{1}{4}\left(\frac{rn+2r+7n+6}{32n}\right) - \frac{\alpha_r}{16} & \text{if } n \text{ is odd,} \\ \frac{1}{4}\left(\frac{5}{4n} + \frac{r-1}{4(n+2)} + \frac{3-\alpha_r}{4}\right) & \text{if } n \text{ is even,} \quad \text{where } \alpha_r = \sum_{i=2}^{r} i \end{cases}$$

$$(iii)\ \ ID(G) = \begin{cases} \frac{5}{6} & \text{if } n \text{ is odd,} \\ \frac{7}{6} & \text{if } n \text{ is even.} \end{cases}$$

Similarly, the next results can easily proved by using Table 2 and 3. Then

Table 2. The circular ladder graph $CL[n]$ with n cycle.

Vertices	Degree	Eccentricity	Frequency
u	3	$\lceil \frac{n}{2} \rceil + 1$	$2n+2$

Table 3. The mobius ladder graph $ML[n]$ with n cycle.

Vertices	Degree	Eccentricity	Frequency
u	3	$\lceil \frac{n}{2} \rceil$	$2n+2$

Theorem 2.3. Let $G = CL[n]$ be a circular ladder. Then
(i) $\xi_{ce}^{-1}(G) = \frac{2}{3}(nr + r + n + 1)$, where $r = \lceil \frac{n}{2} \rceil$
(ii) $ECP(G,x) = 3x^{2(n+1)(r+1)}$, where $r = \lceil \frac{n}{2} \rceil$
(iii) $\zeta^{-1}(G) = \frac{1}{2(n+1)(r+1)}$, where $r = \lceil \frac{n}{2} \rceil$
(iv) $ID(G) = \frac{1}{3}$.

Theorem 2.4. Let $G = ML[n]$ be a Mobius ladder. Then
(i) $\xi_{ce}^{-1}(G) = \frac{2}{3}(r(n+1))$, where $r = \lceil \frac{n}{2} \rceil$
(ii) $ECP(G,x) = 3x^{2r(n+1)}$, where $r = \lceil \frac{n}{2} \rceil$
(iii) $\zeta^{-1}(G) = \frac{1}{2r(n+1)}$, where $r = \lceil \frac{n}{2} \rceil$
(iv) $ID(G) = \frac{1}{3}$.

We calculate the inverse connective eccentricity index, the eccentricity connectivity polynomial index, the inverse total eccentricity index and the inverse degree index of the line graphs of the $L[n]$, $CL[n]$ and ML[n]. In Table 4-6, we present these vertices for each graph along with their degrees, eccentricities and frequency.

Table 4. The ladder graph $\Gamma(L[n])$ with n cycle.

Vertices	Degree	Eccentricity	Frequency
u_1	3	n	4
$u_i(2 \leq i \leq \frac{n}{2}, n \text{ is even})$	4	$n-i+1$	4
$u_i(2 \leq i < \lceil \frac{n}{2} \rceil, n \text{ is odd})$	4	$n-i+1$	4
$u_{\lceil \frac{n}{2} \rceil}(n \text{ is odd})$	4	$\frac{n+1}{2}$	2
w_1	2	$n+1$	2
$w_i(2 \leq i \leq \frac{n}{2}, n \text{ is even})$	4	$n-i+2$	2
$w_i(2 \leq i < \lceil \frac{n}{2} \rceil, n \text{ is odd})$	4	$n-i+2$	2
$w_{\frac{n}{2}+1}(n \text{ is even})$	4	$\frac{n+2}{2}$	1
$w_{\lceil \frac{n}{2} \rceil}(n \text{ is odd})$	4	$\frac{n+3}{2}$	2

Theorem 2.5. Let n be a positive integer. Then inverse connective eccentricity index of a graph $G = \Gamma(L[n])$ is

$$\xi_{ce}^{-1}(G) = \begin{cases} \frac{6nr-r^2+9r+n-3}{4} & \text{if } n \text{ is odd,} \\ \frac{n(9r+5)}{6} - \frac{3r(r-3)}{4} + 1 & \text{if } n \text{ is even.} \end{cases}$$

Proof: The proof is given for parity of n, that is , odd and even. By the definition inverse connective eccentricity,

$$\xi_{ce}^{-1}(G) = \sum_{u \in V(G)} \frac{\epsilon_G(u)}{d_G(u)}.$$

By Table 4, and if n is odd, we have

$$\begin{aligned} \xi_{ce}^{-1}(G) &= \frac{4n}{3} + \sum_{i=2}^{r}(n+1-i) + \frac{n+1}{2} + \frac{\sum\limits_{i=2}^{r}(n+2-i)}{2} + \frac{n+3}{4} \\ &= \frac{6nr-r^2+9r+n-3}{4}. \end{aligned}$$

By Table 4, and if n is even, we have

$$\begin{aligned} \xi_{ce}^{-1}(G) &= \frac{4n}{3} + \sum_{i=2}^{r}(n+1-i) + (n+1) + \frac{\sum\limits_{i=2}^{r}(n+2-i)}{2} \\ &= \frac{n(9r+5)}{6} - \frac{3r(r-3)}{4} + 1. \end{aligned}$$

Corollary 2.6. Let $G = \Gamma(L[n])$. Then

$$(i)\ \ ECP(G,x) = \begin{cases} 2x^{2(n+1)} + 3x^{4n} + 4x^{3r(2n-r-1)-5(n-3)} & \text{if } n \text{ is odd,} \\ 2x^{2(n+1)} + 3x^{4n} + 4x^{3r(2n-r-1)-\frac{11n}{2}+13} & \text{if } n \text{ is even.} \end{cases}$$

$$(ii)\ \ \zeta^{-1}(G) \leq \begin{cases} \frac{3r(3-2n)+82n-159-36n\alpha_r}{192n} & \text{if } n \text{ is odd,} \\ \\ \frac{2nr+3r+94n+221-48\alpha_r}{64n} & \text{if } n \text{ is even,} \qquad \text{where } \alpha_r = \sum_{i=2}^{r} i. \end{cases}$$

$$(iii)\ \ ID(G) = \begin{cases} \frac{19}{12} & \text{if } n \text{ is odd,} \\ \frac{11}{6} & \text{if } n \text{ is even.} \end{cases}$$

Table 5. The circular ladder graph $\Gamma(CL[n])$ with n cycle.

Vertices	Degree	Eccentricity	Frequency
u	4	$\lceil \frac{n}{2} \rceil + 1$	$2n+2$
w	4	$\lceil \frac{n}{2} \rceil + 1$	$n+1$

Table 6. The mobius ladder graph $\Gamma(ML[n])$ with n cycle.

Vertices	Degree	Eccentricity	Frequency
u	4	$\lfloor \frac{n}{2} \rfloor + 1$	2n+2
w	4	$\lfloor \frac{n}{2} \rfloor + 2$	n+1

The next results can be proved by using Table 5 and Table 6, we get

Theorem 2.7. Let $G = \Gamma(CL[n])$ be a circular ladder graph. Then
(i) $\xi_{ce}^{-1}(G) = \frac{3}{4}(n+1)(r+1)$, where $r = \lceil \frac{n}{2} \rceil$.
(ii) $ECP(G,x) = 4x^{(r+1)(n+1)}(x^2+1)$, where $r = \lceil \frac{n}{2} \rceil$.
(iii) $\zeta^{-1}(G) = \frac{3}{2(r+1)(n+1)}$, where $r = \lceil \frac{n}{2} \rceil$.
(iv) $ID(G) = \frac{1}{2}$.

Theorem 2.8. Let $G = \Gamma(ML[n])$ be a Mobius Ladder graph. Then
(i) $\xi_{ce}^{-1}(G) = \frac{n+1}{4}(3r+4)$, where $r = \lfloor \frac{n}{2} \rfloor$.
(ii) $ECP(G,x) = 4x^{n(r-1)+r+2}$, where $r = \lfloor \frac{n}{2} \rfloor$.
(iii) $\zeta^{-1}(G) = \frac{1}{n+1}\left(1 + \frac{3}{2r}\right)$, where $r = \lfloor \frac{n}{2} \rfloor$.
(iv) $ID(G) = \frac{1}{2}$.

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