Distance and eccentricity based polynomials and indices of m -level Wheel graph

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Abstract:

Distance and degree based topological polynomial and indices of molecular graphs have various applications in chemistry, computer networking and pharmacy. In this paper, we give hosoya polynomial, Harary polynomial, Schultz polynomial, modified Schultz polynomial, eccentric connectivity polynomial, modified Wiener index, modified hyper Wiener index, generalized Harary index, multiplicative Wiener index, Schultz index, modified Schultz index, eccentric connectivity index of generalized wheel networks $W_{n,m}$. We also give pictorial representation of computed topological polynomials and indices on the involved parameters m and n .

Keywords: Hosoya polynomial; Harary polynomial; Schultz polynomial; Eccentric connectivity polynomial; Wiener index; Schultz index; Eccentric connectivity index; m -level wheel graph.

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1. Introduction

A simple graph $G = (V, E)$ is a finite nonempty set $V(G)$ of objects called vertices together with a (possibly empty) set $E(G)$ of unordered pairs of distinct vertices of G called edges.

A topological index is a numerical quantity derived in an unambiguous manner from the structure graph of a molecule. As a graph structural invariant, i.e. it does not depend on the labeling or the pictorial representation of a graph. Various topological indices usually reflect molecular size and shape.

The Hosoya polynomial of a graph is a generating function about distance distributing, introduced by Haruo Hosoya in 1998 [17] and for a connected graph G is defined as:

$$H(G, x) = \frac{1}{2} \sum_{v \in V(G)} \sum_{u \in V(G)} x^{d(v,u)},$$

where $d(u, v)$ denotes the distance between vertices u and v .

The Hosoya polynomial has many chemical applications [16] especially Wiener index can be directly obtained from the polynomial and studied extensively [9,10,26].

The main advantage of the Hosoya polynomial is that it contains a wealth of information about distance based graph invariants. For instance, knowing the Hosoya polynomial of a graph, it is straight forward to determine the famous Wiener index of a graph as the first derivative of the polynomial.

The Wiener index of a connected graph G is denoted by $W(G)$ and defined as the sum of distances between all pairs of vertices in G i.e.

$$W(G) = \frac{1}{2} \sum_{v \in V(G)} \sum_{u \in V(G)} d(u, v).$$

The modified Wiener index of a connected graph G is denoted by $W_\lambda(G)$ and defined as the sum of λ power distances between all pairs of vertices in G , where $\lambda = \{1, 2, 3, 4, \dots\}$. It can be formulated as

$$W_\lambda(G) = \frac{1}{2} \sum_{v \in V(G)} \sum_{u \in V(G)} d(u, v)^\lambda$$

The Wiener index was introduced by Harold Wiener in 1947 to study the boiling points of paraffin [31]. It plays an important role in the so-called inverse structure-property relationship problems [11]. For more details about

this topological polynomial and index, please see the paper series and the references therein [3,6,15,23,27,30]. Note that the first derivative of the Hosoya polynomial at $x = 1$ is equal to the Wiener index:

$$W(G) = \left. \frac{\partial H(g)}{\partial x} \right|_{x=1}$$

Hyper-Wiener index is another distance-based graph invariants used for predicting physico-chemical properties of organic compounds [20]. The Hyper-Wiener index was introduced by M. Randić [31] as:

$$WW(G) = \frac{1}{2} \sum_{v \in V(G)} \sum_{u \in V(G)} (d(u, v) + d(u, v)^2).$$

Modified Hyper Wiener index of a connected graph G is denoted by $WW_\lambda(G)$ and defined as:

$$WW_\lambda(G) = \frac{1}{2} \sum_{v \in V(G)} \sum_{u \in V(G)} (d(u, v)^\lambda + d(u, v)^{2\lambda}).$$

where $\lambda = \{1, 2, 3, 4, \dots\}$

The Schultz index of a molecular graph G was introduced by Schultz [22] in 1989 for characterizing alkanes by an integer as follow:

$$Sc(G) = \frac{1}{2} \sum_{v \in V(G)} \sum_{u \in V(G)} (d_u + d_v)d(u, v)$$

The modified Schultz index of a graph G was introduced by S. Klavár and I. Gutman in 1996 as follow [18]:

$$Sc^*(G) = \frac{1}{2} \sum_{v \in V(G)} \sum_{u \in V(G)} (d_u d_v)d(u, v).$$

The Schultz and modified Schultz polynomials of G are defined as [4]:

$$Sc(G) = \frac{1}{2} \sum_{v \in V(G)} \sum_{u \in V(G)} (d_u + d_v)x^{d(u, v)}$$

$$Sc^*(G) = \frac{1}{2} \sum_{v \in V(G)} \sum_{u \in V(G)} (d_u d_v)x^{d(u, v)}$$

The Harary polynomial of a connected graph G is denoted by $h(G, x)$ and defined as

$$h(G, x) = \frac{1}{2} \sum_{v \in V(G)} \sum_{u \in V(G)} \frac{1}{d(v, u)} x^{d(v, u)},$$

The generalized Harary index of a connected graph G is denoted by $h_t(G)$ and defined as

$$h_t(G) = \sum_{v \in V(G)} \sum_{u \in V(G)} \frac{1}{d(v, u) + t}$$

The multiplicative Wiener index of a connected graph G is denoted by $\pi(G)$ and defined as

$$\pi(G) = \prod_{u, v \in V(G)} d(u, v)$$

The eccentricity $ec(v)$ of vertex $v \in V(G)$ is the maximum distance between v and any other vertex in G . Then the eccentric connectivity index (ECI) of G was introduced by Sharma and Madan [24] as

$$\xi(G) = \sum_{v \in V(G)} \sum_{u \in V(G)} d(v, u) \varepsilon(v)$$

As the extension of eccentric connectivity index, eccentric connectivity polynomial was introduced by Ashraf and Jalali [5] which was denoted as

$$\xi(G, x) = \sum_{v \in V(G)} \sum_{u \in V(G)} d(v, u) x^{\varepsilon(v)}$$

The wheel graph has been used in different areas such as the wireless sensor networks and the vulnerability of networks [7]. The wheel graph has many good properties. From the standpoint of the hub vertex, all elements, including vertices and edges, are in its one-hop neighborhood, which indicates that the wheel structure is fully included in the neighborhood graph of the hub vertex. Wheel and related graphs are extensively studied recently. In [28], the authors computed partition dimension and connected partition dimension of wheel graphs. In [29], the authors gave an algorithm to compute average lower two-domination number and also computed this number for some wheel related graphs. In [25], authors computed the metric dimension of generalised wheel. For more details see [2,19,21,30]. For detailed applications of our results we refer [1,8,12,13,14] and references therein.

In this report, we study Hosoya polynomial, Harary polynomial, Schultz polynomial, modified Schultz polynomial, eccentric connectivity polynomial, modified Wiener index, modified hyper Wiener index, generalized harary index, multiplicative Wiener index, Schultz index, modified Schultz index and eccentric connectivity index of multi-level wheel graph.

2. Main Results

Definition 1 (*m*–level wheel graph). Generalized wheel graph, also known as multi-level wheel network, $W_{m,n}$. An multi-level wheel network $W_{m,n}$ is a network obtained from m –copies of cycles C_n and one copy of vertex v , such that all vertices of every copy of C_n are adjacent to v . Thus, $W_{m,n}$ has $mn + 1$ vertices, i.e. the center and n –rim vertices, and has diameter 2. is shown in figure 1.

Figure 2.1: $W_{4,4}$.

Lemma 1. The graph $W_{m,n}$ having $mn + 1$ vertices and $2mn$ edges.

Theorem 2.1. If $W_{m,n}$ is the m –wheel graph $m \geq 2$, $n \geq 3$, then

$$H(W_{m,n}; x) = mn + 1 + 2mnx + \left(\frac{m^2n^2}{2} - \frac{3mn}{2} \right) x^2$$

Proof. As first term of Hosoya polynomial is number of vertices which can be easily computed by Figure 2.1 $|V(W_n^m)| = mn + 1$. For the second term of Hosoya polynomial is number of edges, central vertex having nm degree and other nm vertex having 3 degree.

$$|E(W_n^m)| = \frac{(mn + 3mn)m}{2} = 2mn$$

For the third term of Hosoya polynomial of W_n^m , we see that the central vertex having only 1-edge paths between all other vertices so remaining mn vertices having 2-edge paths between all other vertices except central vertex i.e mn . So first n vertices of C_n of $W_{m,n}$ having 2-edge paths with all other $(m-1)$ copies of C_n having n vertices, that is $n^2(m-1)$. Similarly second n^2 join with remaining $(m-2)$ copies, i.e $n^2(m-2)$ and so on.

$$\begin{aligned} &= (n)^2(m-1) + (n-1)^2(m-2) + (n-1)^2(m-3) + \dots + (n-1)^2 \cdot 2 + (n-1)^2 \\ &= (n-1)^2[(m-1) + (m-2) + (m-3) + \dots + 2 + 1] \\ &= \frac{n^2m(m-1)}{2} \end{aligned}$$

as wheel graph having $\frac{n^2}{2} - \frac{3n}{2}$, 2-edge paths and generalized wheel graph having m -wheels so m times 2-edge paths i.e $m\left(\frac{n^2}{2} - \frac{3n}{2}\right)$ now, the coefficient of the third term of Hosoya polynomial will be

$$\begin{aligned} &= \frac{n^2m(m-1)}{2} + m\left(\frac{n^2}{2} - \frac{3n}{2}\right) \\ &= \frac{m^2n^2}{2} - \frac{3mn}{2} \end{aligned}$$

Here, by what have been mentioned above, we have following computations for the Hosoya polynomial of m -wheel graph W_n^m .

$$H(W_{m,n}; x) = mn + 1 + 2mnx + \left(\frac{m^2n^2}{2} - \frac{3mn}{2}\right)x^2$$

. $\square$

Table 1. Hosoya polynomial of $(W_{m,n})$			
<i>Distances</i>	0	1	2
Terms of Hosoya polynomial	$mn + 1$	$2mn$	$\frac{m^2n^2}{2} - \frac{3mn}{2}$

Theorem 2.2. For the m -wheel graph $W_{m,n}$, the harary polynomial is

$$h(W_{m,n}; x) = 2mnx + \left(\frac{m^2n^2}{4} - \frac{3mn}{4}\right)x^2$$

Proof. From table 1

$$\begin{aligned}
 h(W_{m,n}, x) &= \sum_{v \in V(W_{m,n})} \sum_{u \in V(W_{m,n})} \frac{1}{d(u, v)} x^{d(u, v)} \\
 &= \sum_{v \in V(W_{m,n})} \sum_{u \in V(W_{m,n})} \frac{1}{1} x^1 + \sum_{v \in V(W_{m,n})} \sum_{u \in V(W_{m,n})} \frac{1}{2} x^2 \\
 h(W_{m,n}; x) &= 2mnx + \left(\frac{m^2 n^2}{4} - \frac{3mn}{4} \right) x^2
 \end{aligned}$$

□

Theorem 2.3. For the m -wheel graph $W_{m,n}$, we have

1. $W_\lambda(W_{m,n}) = 2mn + (m^2 n^2 - 3mn) 2^{\lambda-1}$
2. $WW_\lambda(W_{m,n}) = 4mn + (m^2 n^2 - 3mn)(2^{\lambda-1} + 2^{2\lambda-1})$
3. $h_t(W_{m,n}) = \frac{2mn}{(1+t)} + \frac{m^2 n^2 - 3mn}{2(2+t)}$
4. $\pi(W_{m,n}) = 1^{2mn} \times 2^{\left(\frac{m^2 n^2}{2} - \frac{3mn}{2}\right)}$

Proof. As modified Wiener index is

$$\begin{aligned}
 W_\lambda(W_{m,n}) &= \frac{1}{2} \sum_{v \in V(W_{m,n})} \sum_{u \in V(W_{m,n})} d(u, v)^\lambda \\
 &= \frac{1}{2} \sum_{v \in V(W_{m,n})} \sum_{u \in V(W_{m,n})} (1)^\lambda + \frac{1}{2} \sum_{v \in V(W_{m,n})} \sum_{u \in V(W_{m,n})} (2)^\lambda \\
 &= 2mn + (m^2 n^2 - 3mn) 2^{\lambda-1}
 \end{aligned}$$

In Table 2 modified Wiener index of m -wheel graphs for $n = 9$ and different values of m and λ .

Table 2. Modified Wiener index of $(W_\lambda(W_{m,9}))$						
$\lambda \backslash m$	1	2	3	4	5	6
1	72	306	702	1260	1980	2862
2	126	576	1350	2448	38707	5616
3	234	1116	2646	4824	7650	11124
4	450	2196	5238	9576	15210	22140
5	882	4356	10422	19080	30330	44172
6	1746	8676	20790	38088	60570	88236

For modified Hyper Wiener index

$$\begin{aligned}
 WW_\lambda(W_{m,n}) &= \frac{1}{2} \left(\sum_{v \in V(W_{m,n})} \sum_{u \in V(W_{m,n})} d(u, v)^\lambda + \sum_{v \in V(W_{m,n})} \sum_{u \in V(W_{m,n})} d(u, v)^{2\lambda} \right) \\
 &= W_\lambda(W_{m,n}) + \frac{1}{2} \sum_{v \in V(W_{m,n})} \sum_{u \in V(W_{m,n})} d(u, v)^{2\lambda} \\
 &= W_\lambda(W_{m,n}) + \frac{1}{2} \sum_{v \in V(W_{m,n})} \sum_{u \in V(W_{m,n})} (1)^{2\lambda} \\
 &\quad + \frac{1}{2} \sum_{v \in V(W_{m,n})} \sum_{u \in V(W_{m,n})} (2)^{2\lambda} \\
 &= \frac{1}{2} \sum_{v \in V(W_{m,n})} \sum_{u \in V(W_{m,n})} (1^\lambda + 1^{2\lambda}) \\
 &\quad + \frac{1}{2} \sum_{v \in V(W_{m,n})} \sum_{u \in V(W_{m,n})} (2^\lambda + 2^{2\lambda}) \\
 WW_\lambda(W_{m,n}) &= 4mn + (m^2n^2 - 3mn)(2^{\lambda-1} + 2^{2\lambda-1})
 \end{aligned}$$

In table 3 modified Hyper-Wiener index of m -wheel graphs for $n = 9$ and different values of m and λ .

Table 3. Modified Hyper Wiener index of $(WW_\lambda(W_{m,9}))$						
$\lambda \backslash m$	1	2	3	4	5	6
1	198	882	2052	3708	5850	8478
2	576	2772	6588	12024	19080	27756
height3	1980	9792	23436	42912	68220	99360
4	7380	36792	88236	161712	257220	374760
5	28548	142632	342252	627408	998100	1454328
6	112356	561672	1347948	2471184	3931380	5728536

For generalized harary index

$$\begin{aligned}
 h_t(W_{m,n}) &= \frac{1}{2} \sum_{v \in V(W_{m,n})} \sum_{u \in V(W_{m,n})} \frac{1}{d(u, v) + t} \\
 &= \frac{1}{2} \sum_{v \in V(G)} \sum_{u \in V(G)} \frac{1}{1 + t} + \frac{1}{2} \sum_{v \in V(W_{m,n})} \sum_{u \in V(W_{m,n})} \frac{1}{2 + t} \\
 &= \frac{2mn}{(1 + t)} + \frac{m^2n^2 - 3mn}{2(2 + t)}
 \end{aligned}$$

In table 4 generalized Harary index of m -wheel graphs for $n = 9$ and different values of m and t .

Table 4. generalized Harary index of $(H_t W_{m,9})$						
$t \backslash m$	1	2	3	4	5	6
0	63/2	207/2	216	369	1125/2	1593/2
height1	18	63	135	234	360	513
height2	51/4	183/4	99	345/2	1065/4	1521/4
height3	99/10	36	783/10	684/5	423/2	1512/5
4	81/10	297/10	324/5	567/5	351/2	2511/10
5	48/7	177/7	387/7	678/7	150	1503/7
6	333/56	1233/56	675/14	2367/28	7335/56	10503/56

For Multiplicative Wiener index

$$\begin{aligned}
 \pi(G) &= \prod_{u,v \subseteq V(W_{m,n})} d(u,v) \\
 &= \prod_{u,v \subseteq V(W_{m,n})} (1) \times \prod_{u,v \subseteq V(W_{m,n})} (2) \\
 &= 1^{2mn} \times 2^{\left(\frac{m^2 n^2}{2} - \frac{3mn}{2}\right)}
 \end{aligned}$$

□

Corollary 2.4. The Wiener index of m -wheel graph $W_{m,n}$, ($m \geq 2, n \geq 3$) is

$$W_1(W_{m,n}) = m^2 n^2 - mn.$$

Corollary 2.5. The Hyper-Wiener index of m -wheel graph $W_{m,n}$, ($m \geq 2, n \geq 3$) is

$$WW_1(W_{m,n}) = 3m^2 n^2 - 5mn$$

Corollary 2.6. The Harary index of m -wheel graph $W_{m,n}$, ($m \geq 2, n \geq 3$) is

$$h_0(W_{m,n}) = \frac{m^2 n^2 + 5mn}{4}.$$

Theorem 2.7. If $W_{m,n}$ is the m -wheel graph $m \geq 2, n \geq 3$, then

$$Sc(W_{m,n}; x) = (9mn + m^2 n^2)x + (3m^2 n^2 - 9mn)x^2$$

$$Sc^*(W_{m,n}; x) = (9mn + 3m^2 n^2)x + \left(\frac{9m^2 n^2}{2} - \frac{27mn}{2}\right)x^2.$$

Proof. As $d(u, v) \in \{1, 2\}$ and $d_u = i$, $d_v = j$. To prove these results we need to compute i -th paths and i -th term of Schultz and modified Schultz polynomials as commuted in table 5. The number of i -th component of Schultz polynomial is sum of degrees of corresponding vertices multiplied by total number of i -th paths and the number of i -th component of modified Schultz polynomial is product of degrees of corresponding vertices multiplied by total number of i -th paths.

Table 5. The number of all distinct types of 1 and 2-edge-paths				
i - th edge paths	d_u, d_v	Number of i -th paths	terms of Schultz polynomial	terms of Modified Schultz polynomial
1	3, 3	mn	$6mn$	$9mn$
1	3, m	mn	$(3 + mn)mn$	$3m^2n^2$
2	3, 3	$\frac{m^2n^2}{2} - \frac{3mn}{2}$	$3m^2n^2 - 9mn$	$\frac{9m^2n^2}{2} - \frac{27mn}{2}$

Therefore, the Schultz, Modified Schultz polynomials of the m -level wheel graph $W_{m,n}$ are equal to:

$$\begin{aligned}
 Sc(W_{m,n}, x) &= \frac{1}{2} \sum_{v \in V(G)} (d_u + d_v) x^{d(u,v)} \\
 &= ((6)mn + (3 + mn)mn)x + (6) \left(\frac{m^2n^2}{2} - \frac{3mn}{2} \right) x^2 \\
 &= (9mn + m^2n^2)x + (3m^2n^2 - 9mn)x^2
 \end{aligned}$$

$$\begin{aligned}
 Sc^*(W_{m,n}, x) &= \frac{1}{2} \sum_{v \in V(G)} (d_u d_v) x^{d(u,v)} \\
 &= ((9)mn + (3mn)mn)x + (9) \left(\frac{m^2n^2}{2} - \frac{3mn}{2} \right) x^2 \\
 &= (9mn + 3m^2n^2)x + \left(\frac{9m^2n^2}{2} - \frac{27mn}{2} \right) x^2
 \end{aligned}$$

□

Theorem 2.8. If $W_{m,n}$ is the m -wheel graph $m \geq 2$, $n \geq 3$, then

$$Sc(W_{m,n}) = 7m^2n^2 - 9mn$$

$$Sc^*(W_{m,n}) = 12m^2n^2 - 18mn.$$

Proof. Consider the m -wheel graph $W_{m,n}$ from the definition of Schultz index and the Modified Schultz index of a graph G , we can see the Schultz and Modified Schultz indices of G , by the first derivative of their polynomials (evaluated at $x = 1$). So, by using above mentions results, we have following computations

$$\begin{aligned} Sc(W_{m,n}) &= \frac{\partial Sc(W_{m,n}, x)}{\partial x} \Big|_{x=1} \\ &= \frac{\partial}{\partial x} [(9mn + m^2n^2)x + (3m^2n^2 - 9mn)x^2] \Big|_{x=1} \\ &= 7m^2n^2 - 9mn \end{aligned}$$

$$\begin{aligned} Sc^*(W_{m,n}) &= \frac{\partial Sc^*(W_{m,n}, x)}{\partial x} \Big|_{x=1} \\ &= \frac{\partial}{\partial x} [(9mn + 3m^2n^2)x + (\frac{9m^2n^2}{2} - \frac{27mn}{2})x^2] \Big|_{x=1} \\ &= 12m^2n^2 - 18mn \end{aligned}$$

□

Theorem 2.9. If $W_{m,n}$ is the m -wheel graph $m \geq 2$, $n \geq 3$, then

$$\begin{aligned} \xi(W_{m,n}, x) &= mnx + 3mnx^2 \\ &= 7mn \end{aligned}$$

Proof. Consider the m -wheel graph $W_{m,n}$, this graph has a central vertex such as u , with $ecc(u) = 1$ and other mn vertices say v_i having $ecc(v_i) = 2$ and degrees of u and v_i 's are mn and 3 respectively. By the definition eccentric connectivity polynomial, we have following computations

$$\begin{aligned}
\xi(W_{m,n}, x) &= \sum_{v \in V(W_{m,n})} d(v, u) x^{\varepsilon(v)} \\
&= mnx + 3mnx^2
\end{aligned}$$

the definition of eccentric connectivity index, we can see the eccentric connectivity index of G , by the first derivative of their polynomials (evaluated at $x = 1$). So, by using above mentions results, we have following computations

$$\begin{aligned}
\xi(W_{m,n}) &= \left. \frac{\partial \xi(W_{m,n}, x)}{\partial x} \right|_{x=1} \\
&= \left. \frac{\partial}{\partial x} [mnx + 3mnx^2] \right|_{x=1} \\
&= 7mn.
\end{aligned}$$

□

3. Graphical representation and concluding remarks

In the current article, we computed distances based topological polynomials and indices of multi-level wheels, which are the extension of classical wheel graph. Figure 3.1 shows the comparison of Hosoya polynomial, Harary polynomial, Schultz polynomial, modified Schultz polynomial and eccentric connectivity polynomial with fixed value of m and n i.e $m = 7, n = 12$. Every polynomial is exponentially increasing but modified Schultz is faster and eccentric connectivity is slower. Figure 3.2 depict the mesh plotting and comparison of Wiener index, Hyper Wiener index, Harary index, Schultz index, modified Schultz index and Eccentric connectivity index with $2 \leq m \leq 50, 3 \leq n \leq 50$.

Figure 3.1: Polynomials of $W_{m,n}$ for $m = 7, n = 12$.

Figure 3.2: Indices of $W_{m,n}$ for $2 \leq m \leq 50, 3 \leq n \leq 50$.

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