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Distance-based topological indices of Möbius ladder graphs: a mathematical perspective

S. Shokrollahi Yancheshmeh[a,*], M. Jahandideh Khangheshlaghi[b]

[a] *Department of Mathematics, Ahv.C., Islamic Azad University, Ahvaz, Iran.*
[b] *Department of Mathematics, Mahs.C., Islamic Azad University, Mahshahr, Iran.*

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Abstract. Topological indices—quantitative descriptors of connected graphs—play a pivotal role in mathematical chemistry and network analysis by capturing key structural properties. In this research, a set of well-known distance-based topological indices, including Wiener, Hyper-Wiener, Padmakar–Ivan, Szeged, Gutman and Degree Distance have been computed for the Möbius ladder graph M_n. By employing the automorphism group of the graph, $\mathrm{Aut}(G)$, we derive closed-form expressions for each index for arbitrary n. Detailed comparison for n ranging from 6 to 50, based on mathematical analysis and graphical illustrations, reveals that the Hyper-Wiener index effectively serves as a measure of central tendency and closely approximates the numerical mean of the other indices. Interestingly, the pairs (Wiener, PadmakarIvan) and (Szeged, Degree Distance) exhibit similar growth patterns and numerical behavior. These findings, presented in both tabular and graphical form, highlight the variations and interrelationships among the indices. To the best of our knowledge, this study offers the first systematic computation of distance-based indices for M_n, revealing unique structural features. The comparative analysis not only enriches the understanding of topological indices in graph theory but also opens new avenues for applications in molecular structure modeling and biological network analysis.

Keywords: Möbius ladder, hyper Weiner index, Padmakar-Ivan, degree-distance.

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1. Introduction and preliminaries

Let G be a connected graph that contains neither loops nor multiple edges. A bijective function θ that maps the vertex set $V(G)$ onto itself and preserves adjacency between

*Corresponding author.
E-mail address: shokrolahi1373@gmail.com, sa.shokrollahi@iau.ac.ir (S. Shokrollahi); m.jahandideh.kh@iau.ac.ir (M. Jahandideh).

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vertices is called an automorphism of G. A graph invariant is a numerical characteristic that depends solely on the graphs configuration and remains unchanged under all automorphisms. A notable subclass of graph invariants, known as topological indices, plays a key role in mathematical chemistry. When a graph is used to model a molecular structure, these indices are instrumental in predicting the compounds physical or chemical properties [18, 19].

The Wiener index was first proposed by H. Wiener to estimate the boiling points of paraffins [27]. Its formula is $W(G) = \sum_{\{r,s\}\subseteq V(G)} d(r,s)$, where $d(r,s)$ indicates the minimum number of edges along any path connecting vertices r and s. An equivalent formulation is $W(G) = \frac{1}{2}\sum_{r\in V(G)} d(r)$, where $d(r) = \sum_{x\in V(G)} d(r,x)$ denotes the total distance from vertex r to all other vertices in the graph [10, 12, 16, 28]. Building on this concept, the Hyper-Wiener index, first defined by Randi [24] and later generalized by Klein et al. [23] incorporates both linear and squared distances:

$$WW(G) = \frac{1}{2}\sum_{\{r,s\}\subseteq V(G)} \left[d(r,s)^2 + d(r,s)\right],$$

or equivalently,

$$WW(G) = \frac{1}{2}\left(W(G) + \sum_{\{r,s\}\subseteq V(G)} d^2(r,s)\right).$$

This index captures more complex structural information by assigning greater weight to longer paths [3, 29]. The Degree Distance index (or first Schultz index) [4, 5, 25, 26] combines degree information with distance and is given by

$$DD(G) = \sum_{\{r,s\}\subseteq V(G)} \left(\deg_G(r) + \deg_G(s)\right) d(r,s),$$

where $\deg_G(r)$ is the degree of vertex r. The Gutman index [2, 11, 13, 17] modifies the Schultz index by taking the product of degrees instead of their sum:

$$Gut(G) = \sum_{\{r,s\}\subseteq V(G)} (\deg_G(r)\cdot \deg_G(s)) d(r,s).$$

This formulation is particularly sensitive to highly connected vertices, making it effective for analyzing branching patterns and structural complexity. The Szeged index [7, 8, 14, 15] is expressed as $Sz(G) = \sum_{e=rs\in E(G)} n_r(e|G)\cdot n_s(e|G)$, where $n_r(e|G)$ and $n_s(e|G)$ denote the number of vertices closer to r and s, respectively. These are defined as

$$N_r(e|G) = \{u \in V(G) \mid d(u,r) < d(u,s)\}, \quad n_r(e|G) = |N_r(e|G)|,$$
$$N_s(e|G) = \{u \in V(G) \mid d(u,s) < d(u,r)\}, \quad n_s(e|G) = |N_s(e|G)|.$$

The PadmakarIvan (PI) index [1, 20–22] is another edge-based descriptor defined as

$$PI(G) = \sum_{e=rs\in E(G)} \left(n_{er}(e|G) + n_{es}(e|G)\right),$$

where $n_{er}(e|G)$ and $n_{es}(e|G)$ count the number of edges in the subgraphs induced by $N_r(e|G)$ and $N_s(e|G)$, respectively.

In many cases, the group of Aut(G) can significantly simplify the computation of topological indices.

Definition 1.1 An automorphism of a simple graph G is a permutation θ on $V(G)$ such that for every edge $xy \in E(G)$, the image $\theta(x)\theta(y) \in E(G)$.

Remark 1 *Aut(G) forms a group under composition.*

Definition 1.2 The action of Aut(G) on $V(G)$ is said to be transitive if, for every pair $y, x \in V(G)$, there exists an automorphism $\theta \in \mathrm{Aut}(G)$ such that $\theta(y) = x$. In this case, G is called a vertex-transitive graph.

For a connected graph G, we have the following lemmas:

Lemma 1.3 [6] If the automorphism group Aut(G) partitions $V(G)$ into orbits Δ_i with representatives y_i, then $W(G) = \frac{1}{2}\sum_{i=1}^{k} |\Delta_i| d(r_i)$, where $d(r_i) = \sum_{x \in V(G)} d(r_i, x)$. If G is vertex-transitive, then $W(G) = \frac{1}{2}|V(G)|d(r)$ for any $r \in V(G)$.

Lemma 1.4 [6] If Aut(G) partitions $E(G)$ into orbits E_i with representatives $e_i = r_i s_i$,

$$Sz(G) = \sum_{i=1}^{k} |E_i| \cdot n_{r_i}(e_i|G) \cdot n_{s_i}(e_i|G) \text{ and } PI(G) = \sum_{i=1}^{k} |E_i| \cdot \big(n_{er_i}(e_i|G) + n_{es_i}(e_i|G)\big).$$

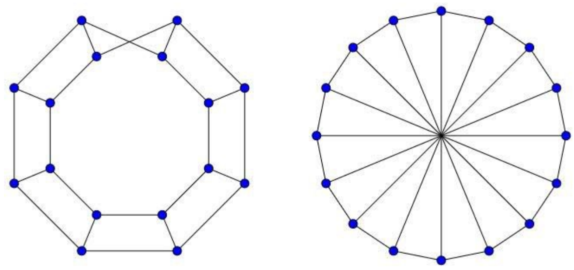
The Möbius ladder M_n is a special type of cubic graph that can be seen as a variation of the standard ladder graph, enhanced by additional edges that introduce non-planarity and a Möbius-like topology. It consists of $2k$ vertices arranged in two parallel cycles resembling a ladder, with adjacent vertices in each cycle connected by rungs. Unlike the ordinary ladder graph, however, the Möbius ladder incorporates twisted connectionsopposite vertices are joined via crossing edges instead of direct linksforming a structure reminiscent of a Möbius strip, which gives the graph its name. Beyond its intriguing topological structure, the Möbius ladder has found applications across various scientific fields. It is extensively used in modeling chemical molecules, particularly in the study of benzenoid and cyclic compounds with conjugated bonds. Moreover, it plays an important role in cryptography and electronic circuit design, where specific symmetry and connectivity characteristics are essential. In quantum graph theory, the Möbius ladder is employed to analyze spectral properties, further underscoring its significance in mathematical and computational research.

In this study, we compute the Wiener, Hyper-Wiener, Degree Distance, Gutman, Szeged and PadmakarIvan indices for the Möbius ladder graph and derive their closed-form expressions. Furthermore, we perform a comparative analysis of these indices.

2. Calculation of some distance-based indices of M_n

Lemma 2.1 M_n is vertex-transitive.

Proof. Based on Figure 1 (b), the Möbius ladder graph M_n can be represented as a polygonal structure. This implies that its automorphism group contains a cyclic subgroup $\langle 1, 2, 3, \ldots, n\rangle$, ensuring that M_n is vertex-transitive (Definition 1.2). ■



a. b.

Figure 1. Two different representations of M_n

Theorem 2.2 The Wiener index of M_n, $|V(M_n)| = n$ for $n > 4$, is

$$W(M_n) = \begin{cases} \frac{1}{2}n\left(\left(\frac{n}{2}\right)\left(\frac{n+4}{4}\right) - 1\right), & n = 4k, \\ \frac{1}{2}n\left(\frac{(n+2)^2}{8} - 1\right), & n = 4k+2. \end{cases}$$

Proof. According to Lemma 1.3 and Lemma 2.1, we have

$$W(M_n) = \frac{1}{2}nd(x_1). \tag{1}$$

The value of $d(x_i)$ is computed in two separate cases: $n = 4k$ and $n = 4k+2$. We consider x_1 as a representative vertex from the vertex set and $d(x_1) = \sum_{i=2}^{n} d(x_1, x_i)$. There are two distinct cases.

Case 1: $n = 4k$. As M_n is symmetric, we have $d(x_1, x_i) = i - 1$ for $2 \leqslant i \leqslant \frac{n}{4} + 1$ and

$$\sum_{i=\frac{n}{4}+2}^{\frac{n}{2}+1} d(x_1, x_i) = \sum_{i=2}^{\frac{n}{4}+1} d(x_1, x_i), \quad \sum_{i=\frac{n}{2}+2}^{n} d(x_1, x_i) = \sum_{i=2}^{\frac{n}{2}} d(x_1, x_i).$$

Thus,

$$\begin{aligned} \sum_{i=\frac{n}{2}+2}^{n} d(x_1, x_i) = \sum_{i=2}^{\frac{n}{2}} d(x_1, x_i) &= \sum_{i=2}^{\frac{n}{4}+1} d(x_1, x_i) + \sum_{i=\frac{n}{4}+2}^{\frac{n}{2}} d(x_1, x_i) \\ &= 2\sum_{i=2}^{\frac{n}{4}+1} d(x_1, x_i) - d\left(x_1, x_{\frac{n}{2}+1}\right) = 2\sum_{i=2}^{\frac{n}{4}+1} d(x_1, x_i) - 1. \end{aligned}$$

Therefore,

$$\begin{aligned} d(x_1) = \sum_{i=2}^{n} d(x_1, x_i) &= \sum_{i=2}^{\frac{n}{4}+1} d(x_1, x_i) + \sum_{i=\frac{n}{4}+2}^{\frac{n}{2}+1} d(x_1, x_i) + \sum_{i=\frac{n}{2}+2}^{n} d(x_1, x_i) \\ &= 4\sum_{i=1}^{\frac{n}{4}} i - 1 = \frac{n}{2}\left(\frac{n+4}{4}\right) - 1. \end{aligned}$$

Case 2: $n = 4k+2$. We have $d(x_1, x_i) = i - 1$ for $2 \leqslant i \leqslant \frac{n-2}{4} + 2$ and

$$\sum_{i=\frac{n-2}{4}+3}^{\frac{n}{2}+1} d(x_1, x_i) = \sum_{i=2}^{\frac{n-2}{4}+1} d(x_1, x_i), \quad \sum_{i=\frac{n}{2}+2}^{n} d(x_1, x_i) = \sum_{i=2}^{\frac{n}{2}} d(x_1, x_i).$$

Consequently,

$$\begin{aligned}\sum_{i=\frac{n}{2}+2}^{n} d(x_1, x_i) = \sum_{i=2}^{\frac{n}{2}} d(x_1, x_i) &= \sum_{i=2}^{\frac{n-2}{4}+2} d(x_1, x_i) + \sum_{i=\frac{n-2}{4}+3}^{\frac{n}{2}} d(x_1, x_i) \\ &= 2\sum_{i=2}^{\frac{n-2}{4}+1} d(x_1, x_i) + d\left(x_1, x_{\frac{n-2}{4}+2}\right) - d\left(x_1, x_{\frac{n}{2}+1}\right).\end{aligned}$$

So,

$$d(x_1) = 4\sum_{i=1}^{\frac{n-2}{4}} i + 2\left(\frac{n-2}{4} + 1\right) - 1 = \frac{(n+2)^2}{8} - 1.$$

By substituting $d(x_1)$ into (1), the proof is complete. ■

Theorem 2.3 The Hyper-Wiener index of M_n, $|V(M_n)| = n$ for $n > 4$, is

$$WW(M_n) = \begin{cases} \dfrac{n^2(n+4)(n+8)}{192} - \dfrac{n}{2}, & \text{if } n = 4k, \\ \dfrac{n(n+2)(n^2+10n+24)}{192} - \dfrac{n}{2}, & \text{if } n = 4k+2. \end{cases}$$

Proof. According to the formulation of the Hyper-Wiener index:

$$WW(M_n) = \frac{1}{2}\left(W(M_n) + \sum_{\{u,v\}\subset V(M_n)} d^2(u,v)\right). \tag{2}$$

The graph M_n is vertex-transitive (Lemma 2.1). Consequently, any vertex x_1 of the vertex set $V(M_n)$ can be chosen as a representative. Thus, the following relation holds:

$$\sum_{\{u,v\}\subset V(M_n)} d^2(u,v) = \frac{1}{2}|M_n| d^2(x_1) = \frac{1}{2} n d^2(x_1).$$

Now two possible cases are considered.

Case 1: $n = 4k$. Based on Theorem 2.2, we have $d(x_1, x_i) = (i-1)$ for $2 \leqslant i \leqslant \frac{n}{4} + 1$ and

$$\sum_{i=\frac{n}{4}+2}^{\frac{n}{2}+1} d^2(x_1, x_i) = \sum_{i=2}^{\frac{n}{4}+1} d^2(x_1, x_i), \quad \sum_{i=\frac{n}{2}+2}^{n} d^2(x_1, x_i) = \sum_{i=2}^{\frac{n}{2}} d^2(x_1, x_i).$$

Thus, $d^2(x_1, x_i) = (i-1)^2$ for $2 \leqslant i \leqslant \frac{n}{4}+1$ and

$$\sum_{i=\frac{n}{4}+2}^{\frac{n}{2}+1} d^2(x_1, x_i) = \sum_{i=2}^{\frac{n}{4}+1} d^2(x_1, x_i), \quad \sum_{i=\frac{n}{2}+2}^{n} d^2(x_1, x_i) = \sum_{i=2}^{\frac{n}{2}} d^2(x_1, x_i).$$

So,

$$\begin{aligned}\sum_{i=\frac{n}{2}+2}^{n} d^2(x_1, x_i) &= \sum_{i=2}^{\frac{n}{2}} d^2(x_1, x_i) = \sum_{i=2}^{\frac{n}{4}+1} d^2(x_1, x_i) + \sum_{i=\frac{n}{4}+2}^{\frac{n}{2}} d^2(x_1, x_i) \\ &= 2\sum_{i=2}^{\frac{n}{4}+1} d^2(x_1, x_i) - d^2\left(x_1, x_{\frac{n}{2}+1}\right) = 2\sum_{i=2}^{\frac{n}{4}+1} d^2(x_1, x_i) - 1.\end{aligned}$$

Therefore,

$$\begin{aligned}d^2(x_1) &= \sum_{i=2}^{n} d^2(x_1, x_i) = \sum_{i=2}^{\frac{n}{4}+1} d^2(x_1, x_i) + \sum_{i=\frac{n}{4}+2}^{\frac{n}{2}+1} d^2(x_1, x_i) + \sum_{i=\frac{n}{2}+2}^{n} d^2(x_1, x_i) \\ &= 4\sum_{i=2}^{\frac{n}{4}+1} d^2(x_1, x_i) - 1 = 4\sum_{i=1}^{\frac{n}{4}} i^2 - 1 = \frac{n(n+4)(n+2)}{48} - 1\end{aligned}$$

and

$$\sum_{\{u,v\}\subset V(M_n)} d^2(u, v) = \frac{1}{2} n d^2(x_1) = \frac{n}{2}\left(\frac{n(n+4)(n+2)}{48} - 1\right).$$

Case 2: $n = 4k + 2k$. We have $d(x_1, x_i) = i - 1$ for $2 \leqslant i \leqslant \frac{n-2}{4} + 2$. Hence,

$$\sum_{i=\frac{n-2}{4}+3}^{\frac{n}{2}+1} d(x_1, x_i) = \sum_{i=2}^{\frac{n-2}{4}+1} d(x_1, x_i), \quad \sum_{i=\frac{n}{2}+2}^{n} d(x_1, x_i) = \sum_{i=2}^{\frac{n}{2}} d(x_1, x_i)$$

and $d^2(x_1, x_i) = (i-1)^2$ for $2 \leqslant i \leqslant \frac{n-2}{4} + 2$. So,

$$\sum_{i=\frac{n-2}{4}+3}^{\frac{n}{2}+1} d^2(x_1, x_i) = \sum_{i=2}^{\frac{n-2}{4}+1} d^2(x_1, x_i), \quad \sum_{i=\frac{n}{2}+2}^{n} d^2(x_1, x_i) = \sum_{i=2}^{\frac{n}{2}} d^2(x_1, x_i).$$

Therefore,

$$d^2(x_1) = \frac{(n+2)(n^2+4n+12)}{48} - 1, \sum_{\{u,v\}\subset V(M_n)} d^2(u, v) = \frac{n}{2}\left(\frac{(n+2)(n^2+4n+12)}{48} - 1\right).$$

Thus, in either case, substituting into (2), the claim follows. ■

Proposition 2.4 Let M_n be a Möbius ladder graph for $n > 4$.

(a) The Degree-Distance index is

$$DD(M_n) = \begin{cases} 3n\left(\frac{n}{2}\cdot\frac{n+4}{4} - 1\right), & \text{if } n = 4k, \\ 3n\left(\frac{(n+2)^2}{8} - 1\right), & \text{if } n = 4k+2. \end{cases}$$

(b) The Gutman index is

$$\text{Gut}(M_n) = \begin{cases} \frac{9}{2}n\left(\frac{n}{2}\cdot\frac{n+4}{4} - 1\right), & \text{if } n = 4k, \\ \frac{9}{2}n\left(\frac{(n+2)^2}{8} - 1\right), & \text{if } n = 4k+2. \end{cases}$$

Proof. Since each vertex in the Möbius ladder graph M_n has degree 3, the graph is 3-regular. Based on this property, the Degree-Distance and the Gutman indices of M_n are obtained as follows:

$$(a)\ DD(M_n) = \sum_{\{u,v\}\subseteq V(M_n)} (\deg_G(u)+\deg_G(v)d(u,v) = 6\cdot \sum_{\{u,v\}\subseteq V(M_n)} d(u,v) = 6\cdot W(M_n).$$

$$(b)\ \text{Gut}(M_n) = \sum_{\{u,v\}\subseteq V(M_n)} (\deg_G(u)\cdot\deg_G(v))d(u,v) = 9\cdot \sum_{\{u,v\}\subseteq V(M_n)} d(u,v) = 9\cdot W(M_n).$$

By Theorem 2.2, the result follows. ■

Proposition 2.5 Let M_n be a Möbius ladder graph for $n > 4$. The Szeged index of M_n is

$$Sz(M_n) = \begin{cases} \frac{3}{2}n\left(\frac{n}{2} - 1\right)^2, & \text{if } n = 4k, \\ \frac{3}{8}n^3, & \text{if } n = 4k+2. \end{cases}$$

Proof. Given that $|E(M_n)| = \frac{3}{2}|V(M_n)| = \frac{3}{2}n$, and by applying Lemma 1.4, every edge $e = uv$ in M_n can be classified into one of two cases.

Case 1: $n = 4k$. In this case, there exist exactly two vertices whose distances from both u and v are equal to $\frac{n}{4}$. Therefore, $|N_u(e|M_n)| = |N_v(e|M_n)| = \frac{n}{2} - 1$ and

$$Sz(M_n) = \sum_{e=uv\in E(M_n)} (n_u(e|M_n)\cdot n_v(e|M_n)) = \frac{3}{2}n\left(\frac{n}{2} - 1\right)^2.$$

Case 2: $n = 4k+2$. In this case, there is no vertex equidistant from both u and v. Hence, $|N_u(e|M_n)| = |N_v(e|M_n)| = \frac{n}{2}$ and

$$Sz(M_n) = \sum_{e=uv\in E(M_n)} (n_u(e|M_n)\cdot n_v(e|M_n)) = \frac{3}{2}n\left(\frac{n}{2}\right)^2 = \frac{3}{8}n^3.$$

This concludes the proof. ■

Proposition 2.6 Let M_n be a Möbius ladder graph for $n > 6$. The PadmakarIvan index of M_n is

$$PI(M_n) = \begin{cases} 2n(n-5), & \text{if } n = 4k, \\ 2n(n-3), & \text{if } n = 4k+2. \end{cases}$$

Proof. The edge set of M_n includes cycle connections and rung edges, denoted by E_1 and E_2 respectively (see Figure 1 (b)). So, $Aut(M_n)$ on E has two orbits E_1 and E_2 with representatives e_1, e_2 respectively, where $e_i = u_iv_i \in E_i$, $i = 1, 2$.

For every edge $e = uv \in E(M_n)$, as stated in Proposition 2.5:

$$|N_u(e_1|M_n)| = |N_v(e_2|M_n)| = \frac{n}{2} - 1, \quad n = 4k,$$
$$|N_u(e_1|M_n)| = |N_v(e_2|M_n)| = \frac{n}{2}, \quad n = 4k+2.$$

We have two possible cases:

Case 1: $n = 4k$. Subgraphs induced by $N_u(e_1|M_n)$, $N_v(e_1|M_n)$, $e_1 \in E_1$, and similarly for $e_2 \in E_2$ give

$$|N_{e_1u}(e_1|M_n)| = |N_{e_1v}(e_1|M_n)| = \frac{n}{2} - 2,$$
$$|N_{e_2u}(e_2|M_n)| = |N_{e_2v}(e_2|M_n)| = \frac{3}{2}\left(\frac{n}{2} - 2\right) - 1.$$

Then

$$\begin{aligned} PI(M_n) &= 2|E_1|\left(\frac{n}{2} - 2\right) + 2|E_2|\left(\frac{3}{2}\left(\frac{n}{2} - 2\right) - 1\right) \\ &= \frac{n}{2}(n-4) + 2n\left(\frac{3n}{4} - 4\right) = 2n(n-5). \end{aligned}$$

Case 2: $n = 4k+2$. By replacing $\frac{n}{2} - 1$ with $\frac{n}{2}$ and adjusting accordingly,

$$\begin{aligned} PI(M_n) &= 2|E_1|\left(\frac{n}{2} - 1\right) + 2|E_2|\left(\frac{3}{2}\left(\frac{n}{2} - 1\right) - 1\right) \\ &= n\left(\frac{n}{2} - 1\right) + 2n\left(\frac{3}{2}\left(\frac{n}{2} - 1\right) - 1\right) = 2n(n-3). \end{aligned}$$

Therefore, the claim is established. ■

In the following, the values of these indices for the range n from 6 to 50 are presented in a table, and their scatter plot is illustrated. This allows for intuitive and comprehensive comparison and analysis of the data. The lines connecting the data points in the graphs are intended solely to improve visualization of the growth trends. It is evident that these indices are not defined for non-integer or odd values of n.

Table 1.

Index values for Möbius Ladder Graph M_n for $6 \leqslant n \leqslant 50$

n	$W(M_n)$	$WW(M_n)$	$Gut(M_n)$	$DD(M_n)$	$Sz(M_n)$	$PI(M_n)$
6	21	27	189	126	81	36
8	44	60	396	264	108	48
10	85	135	765	510	375	140
12	138	234	1242	828	450	168
14	217	413	1953	1302	1029	308
16	312	632	2808	1872	1176	352
18	441	981	3969	2646	2187	540
20	590	1390	5310	3540	2430	600
22	781	1991	7029	4686	3993	836
24	996	2676	8964	5976	4356	912
26	1261	3627	11349	7566	6591	1196
28	1554	4690	13986	9324	7098	1288
30	1905	6105	17145	11430	10125	1620
32	2304	8640	20736	13824	11520	1920
34	2701	10413	24309	16206	14161	2252
36	3132	12492	28224	18816	16992	2608
38	3605	14883	32445	21630	20089	2988
40	4120	17600	36960	24640	23440	3392
42	4681	20667	41769	27846	27061	3820
44	5288	24108	46872	31248	30976	4272
46	5945	27947	52269	34830	35161	4748
48	6652	32208	57960	38640	39600	5248
50	7415	36915	63945	42630	44325	5772

3. Conclusion

In this paper, we derived general formulas for several topological indices of the Möbius ladder graph and analyzed their growth behavior. To enhance understanding, we computed and visualized these indices for n ranging from 6 to 50, revealing distinct growth patterns (Table 2, Figure 2). Among these indices, the PadmakarIvan index exhibits quadratic growth, whereas the Wiener, Szeged, Gutman, and Degree-Distance indices demonstrate cubic growth, with the Gutman index increasing the fastest. The Hyper-Wiener index follows a quartic growth pattern due to the presence of higher-order terms. Notably, the Wiener and PadmakarIvan indices display similar growth behaviors, indicating a strong correlation, while the Szeged and Degree-Distance indices exhibit

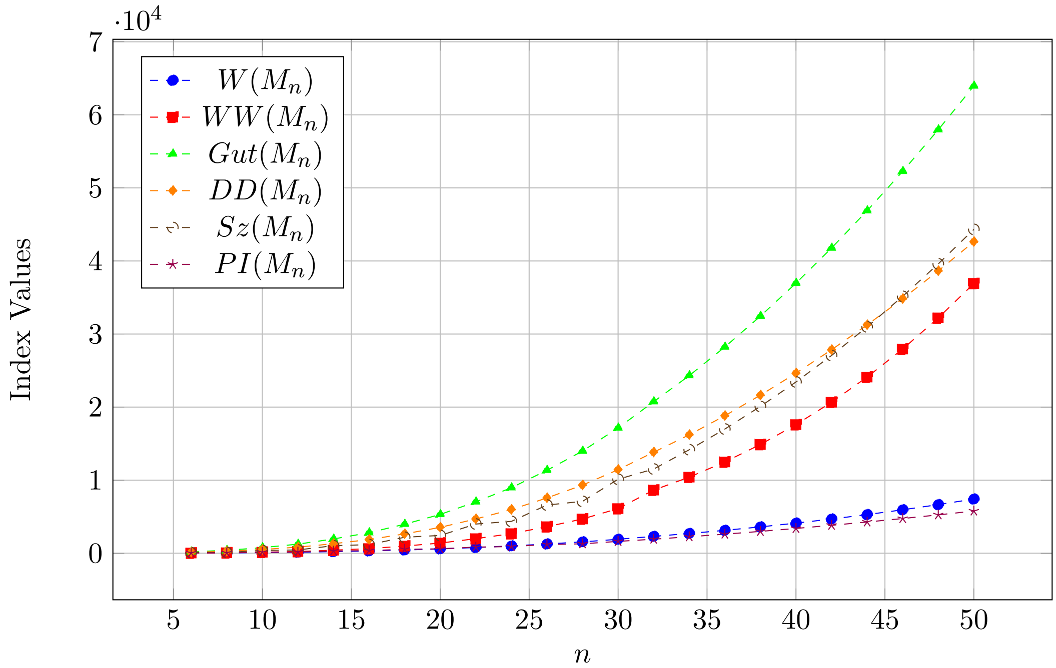


Figure 2. Growth trends of the Distance-Based Indices of M_n

closely aligned trends. The Hyper-Wiener index represents an intermediate growth trajectory, suggesting that the Wiener and PadmakarIvan indices may serve as lower bounds, whereas the Szeged, Degree-Distance, and Gutman indices function as upper bounds.

These observations emphasize the hierarchical impact of graph connectivity and vertex interactions on index values. Further statistical correlation analysis could help quantify these relationships, while comparative visualizations reinforce observed trend similarities. Such insights contribute to advancements in chemical graph theory, network analysis, and complex graph modeling within computational science.

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