

# Analytical Study of Distance-Based Indices for Multi-Layered Triangular Snake Graphs with Pharmaceutical Network Applications

Bharat Suthar<sup>1\*</sup>, Ravi Mahla<sup>2</sup>, Dharna Patel<sup>3</sup> and Yachana Modi<sup>4</sup>

<sup>1,2,3,4</sup>Department of Applied Science and Humanities, Parul Institute of Technology, Parul University, Vadodara, Gujarat, India

<sup>1\*</sup>bharat.suthar8718@paruluniversity.ac.in, <sup>2</sup>ravi.mahla41474@paruluniversity.ac.in, <sup>3</sup>dharna.patel8931@paruluniversity.ac.in and <sup>4</sup>yachana.modi21129@paruluniversity.ac.in

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## ABSTRACT

Graph theory offers effective methodologies for analyzing structural properties of complex networks through distance-oriented topological measures. In this work, we establish generalized closed-form expressions for the Wiener index  $W(G)$  and Degree Distance  $D'(G)$  for the Triangular Snake graph family, including Standard, Double, Triple, and Alternate variants. By applying inductive reasoning and systematic distance-sum decomposition, explicit formulas are obtained and verified against universal bounds for connected graphs.

In addition, the derived indices are interpreted within a transport-network framework, where the Wiener index represents average diffusion distance and the Degree Distance measures connectivity-weighted transport intensity. Asymptotic evaluation reveals polynomial growth behavior and scalable diffusion characteristics in multi-layered structures, providing a rigorous mathematical foundation for the analysis and design of structured drug delivery systems.

**Keywords:** Wiener index, Degree distance, Triangular Snake graphs, Graph invariants, Topological extensions, Pharmaceutical Network

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## 1. INTRODUCTION

Graph theory is a branch of mathematics founded in the 18th century by the renowned mathematician Leonhard Euler, who famously solved the 'Seven Bridges of Königsberg' problem. Since then, graph theory has become essential for solving problems across various scientific fields, introducing numerous concepts and measurements. Among these measurements are topological indices, which are formulated to address specific analytical objectives. The Wiener index and degree distance are two of the most significant indices in this domain. It is well-established that the Wiener index of a molecular graph correlates effectively with certain physical and chemical properties of a molecule, such as its boiling point and solubility. Both indices are fundamentally based on the concept of distance. In 1994 as a weighted version of the Wiener index, which was originally put forward in 1947 by H. Wiener [1]. Over the years, many researchers have explored and generalized such indices across different graph types to evaluate network resilience and structural similarity. For instance, the Eccentric and Leap Eccentric Connectivity indices were defined to indicate the resistance of network structures to external attacks, with detailed studies provided by Aytaç and Gölpeç [6]. In a related direction, Ekinçi and Kirlangic [2] investigated super-edge connectivity on Kronecker product graphs to provide insights into network resilience.

Within the context of chemical structure modeling, such graph-based representations are referred to as chemical graphs. One notable index in this area is the Sombor index, which provides insight into structural similarity. Réti et al. [3] derived several lower and upper bounds for the Sombor index across different chemical graphs. Another significant tool is the Mostar index, which is particularly important for measuring the surface area of octane isomers. Ali and Došlić [4] introduced generalized versions of the Mostar index for specific graph types. Furthermore, Dündar and Gürsoy [5] proposed a new index based on vulnerability and connectivity. These studies represent diverse approaches to measuring how connected networks withstand disruptions.

Determining index values in fundamental graph types facilitates the analysis of more complex structures, allowing for the solution of real-world problems and the comparison of different graph classes. While previous research has presented results for basic graph types such as paths, stars, and cycles, there is a need to extend these generalizations to more specialized families. In this article, we investigate the Wiener index and degree distance generalizations for the Triangular Snake graph family. Using inductive and deductive methods, we derive general formulas for Triangular, Double, Triple, and Alternate

\*Author for Correspondence: bharat.suthar8718@paruluniversity.ac.in

Triangular Snake graphs. Finally, we establish that these results adhere to the established topological bounds and minimum-maximum values for distance-based indices .

**2. BASIC CONCEPTS AND INDEX DEFINITIONS**

Let  $G = (V, E)$  represent a finite, connected, and undirected simple graph. The vertex set is denoted by  $V(G)$  and the edge set by  $E(G)$ . The order of  $G$ , denoted by  $N$ , is the number of vertices, and the size, denoted by  $m$ , is the number of edges. Throughout this study, the distance  $d(u, v)$  between two vertices  $u, v \in V(G)$  is defined as the length of the shortest path connecting them. The degree of a vertex  $v$ , denoted  $\text{deg}(v)$ , is the number of edges incident to it.

**2.1 Wiener Index and Degree Distance**

The Wiener index  $W(G)$ , introduced by Harry Wiener in 1947, is one of the earliest and most widely used topological indices in graph theory and chemical graph theory. It is defined as the sum of the shortest path distances between all unordered pairs of vertices in a graph  $G$ [1].

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v)$$

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

A degree-weighted extension of the Wiener index is the Degree Distance, denoted by  $D'(G)$ . This index was introduced by Alexander A. Dobrynin, R. Entringer and Ivan Gutman in 1994 [3]. The degree distance incorporates vertex degrees into the distance calculation and is defined as

$$D'(G) = \sum_{\{u,v\} \subseteq V(G)} [\text{deg}(u) + \text{deg}(v)]d(u, v)$$

where  $\text{deg}(u)$  and  $\text{deg}(v)$  denote the degrees of vertices  $u$  and  $v$ , respectively.

**2.2 Zagreb Indices**

The Zagreb indices are among the earliest degree-based topological descriptors used in chemical graph theory. They were introduced in 1972 by Ivan Gutman and Nenad Trinajstić for the study of molecular branching and structure-property relationships [11].

The First Zagreb Index is defined as

$$M_1(G) = \sum_{u \in V(G)} \text{deg}^2(u)$$

which represents the sum of the squares of the degrees of all vertices in the graph. The Second Zagreb Index is given by

$$M_2(G) = \sum_{uv \in E(G)} \text{deg}(u)\text{deg}(v)$$

where the summation runs over all edges  $uv$  in the graph  $G$ .

**2.3. Molecular Topological Index (MTI)**

The Molecular Topological Index (MTI) was introduced by H. P. Schultz in 1989 as a structural descriptor for molecular graphs [2]. It is defined using the adjacency matrix  $A$ , the distance matrix  $D$ , and the degree vector  $v$  of the graph.

$$MTI(G) = \sum_{i=1}^n [v(A + D)]_i$$

where  $v$  represents the degree sequence vector of the graph.

It has been shown that the molecular topological index is related to the first Zagreb index and the degree distance through the following relationship:

$$MTI(G) = M_1(G) + D'(G)$$

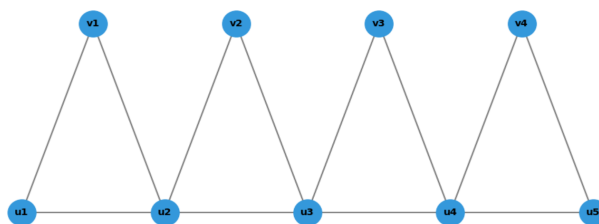
Further studies on these indices and their applications have been carried out by researchers such as Dankelman, Muhammad Ali, and Bucicovschi [16–18].

**3. STRUCTURAL DEFINITIONS**

In this section, we provide the formal structural definitions of the Triangular Snake graph variants analyzed in this study. Each of these graphs is constructed by extending a central path  $P_n$  through the addition of triangular cycles ( $C_3$ ) in specific configurations.

**Definition 3.1: Triangular Snake Graph ( $T_n$ )**

A Triangular Snake graph, denoted  $T_n$ , is obtained from a path  $u_1, u_2, \dots, u_n$  by joining every pair of adjacent vertices  $u_i$  and  $u_{i+1}$  to a new vertex  $v_i$ , for  $i = 1, 2, \dots, n - 1$ . Effectively, each edge of the path  $P_n$  is replaced by a triangular cycle  $C_3$ .



**Figure 1:** Standard Triangular Snake ( $T_n$ )

**Definition 3.2: Double Triangular Snake Graph ( $D(T_n)$ )**

A Double Triangular Snake graph, denoted  $D(T_n)$ , is constructed by taking two triangular snakes that share a

common central path  $u_1, u_2, \dots, u_n$ . In this configuration, each edge  $(u_i, u_{i+1})$  of the path is connected to two distinct apex vertices,  $v_i$  and  $v'_i$ .

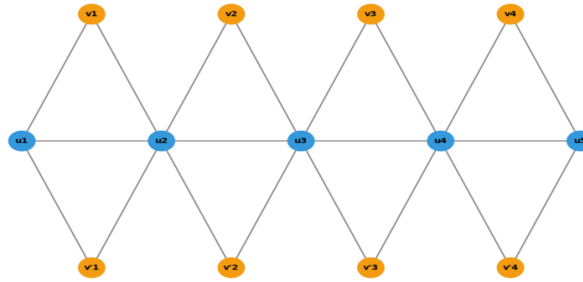


Figure 2: Double Triangular Snake ( $D(T_n)$ )

**Definition 3.3: Triple Triangular Snake Graph ( $T(T_n)$ )** Consequently, each path edge  $(u_i, u_{i+1})$  forms part of three distinct  $C_3$  cycles, connected to apex vertices  $v_i, v'_i,$  and  $v''_i$ .  
 A Triple Triangular Snake graph, denoted  $(T_n)$ , consists of three triangular snakes sharing a common central path.

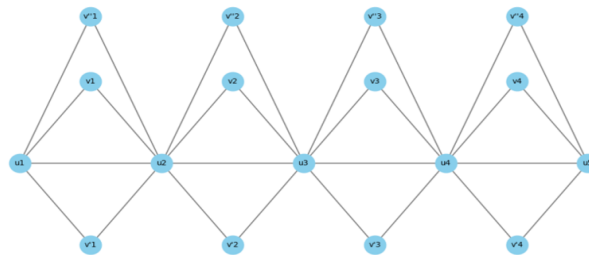


Figure 3: Triple Triangular Snake  $T(T_n)$

**Definition 3.4: Alternate Triangular Snake Graph ( $A(T_n)$ )** a new vertex  $v_i$  for every alternate edge. Specifically, for  $i = 1, 3, 5, \dots$ , the edge  $(u_i, u_{i+1})$  is replaced by a triangular cycle  $C_3$ , while the subsequent edge  $(u_{i+1}, u_{i+2})$  remains a simple path segment.  
 An Alternate Triangular Snake graph, denoted  $A(T_n)$ , is obtained from a path  $u_1, u_2, \dots, u_n$  by joining  $u_i$  and  $u_{i+1}$  to

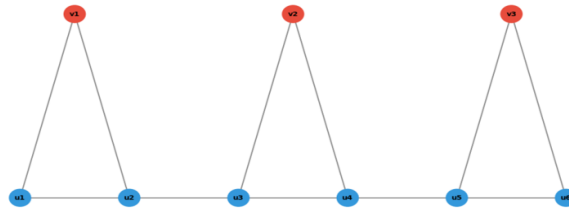


Figure 4: Alternate Triangular Snake  $A(T_n)$

**4. MAIN RESULTS**

In this section, we present the main findings of our study. We derive the general formulas for the Wiener index and degree distance for various members of the Triangular Snake graph family using inductive reasoning and distance-sum partitions.

**Theorem 4.1:** Let  $T_n$  be a Triangular Snake graph of order  $N = 2n - 1$  for  $n \geq 2$ . Then the Wiener index  $W(T_n)$  and the degree distance  $D'(T_n)$  is:

$$W(T_n) = \frac{(n - 1)(2n^2 + 2n - 3)}{3} \tag{4.1.1}$$

$$D'(T_n) = 4(n - 1)^2(n + 1) \tag{4.1.2}$$

**Proof of (4.1.1): Wiener Index**

The Wiener index of a graph  $G$  is defined as:  
 $W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v)$ , where  $d(u,v)$  is the distance between vertices  $u$  and  $v$ . For  $T_n$ , partition the

vertices into: Base path vertices:  $U = \{u_1, u_2, \dots, u_n\}$   
 Apex vertices:  $V_{apex} = \{v_1, v_2, \dots, v_{n-1}\}$

The total Wiener index can be computed as a sum of three parts:

**1. Distances between base vertices ( $W_{uu}$ )**

The base path  $U$  is a simple path  $P_n$ , so the sum of distances is:

$$W_{UU} = \sum_{1 \leq i < j \leq n} |j - i| = \frac{n(n^2 - 1)}{6}$$

**2. Distances between base and apex vertices ( $W_{UV}$ )**

For an apex vertex  $v_i$ :

$$d(v_i, u_j) = \begin{cases} |i - j| & \text{if } j \leq i \\ |j - (i + 1)| + 1 & \text{if } j > i \end{cases}$$

Summing over all apex and base vertices:

$$W_{UV} = \sum_{i=1}^{n-1} \sum_{j=1}^n d(v_i, u_j) = \frac{n(n^2 - 1)}{3}$$

**3. Distances between apex vertices ( $W_{VV}$ )**

For apex vertices  $v_i, v_j (i < j)$ :

$$d(v_i, v_j) = |j - i| + 1$$

Summing over all apex pairs:

$$W_{VV} = \sum_{1 \leq i < j \leq n-1} (|j - i| + 1) = \frac{(n - 1)(n - 2)(n + 3)}{6}$$

Combine all three components

$$W(T_n) = W_{UU} + W_{UV} + W_{VV} = \frac{n(n^2 - 1)}{6} + \frac{n(n^2 - 1)}{3} + \frac{(n - 1)(n - 2)(n + 3)}{6}$$

Simplifying the series and algebra we get

$$D'(T_n) = 4(n - 1)^2(n + 1)$$

**Theorem 4.2:** Let  $G = D(T_n)$  be a Double Triangular Snake graph of order  $N = 3n - 2$  for  $n \geq 2$ . Then the

$$W(D(T_n)) = (n - 1)(n^2 + n + 1) \tag{4.2.1}$$

$$D'(D(T_n)) = \frac{2(n - 1)(11n^2 + 11n - 12)}{3} \tag{4.2.2}$$

**Proof of (4.2.1): Wiener Index**

The Wiener index of a graph  $G$  is:

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v)$$

For  $D(T_n)$ , partition the vertices into three disjoint sets:

- Common path vertices:  $U = \{u_1, u_2, \dots, u_n\}$
- Upper apex vertices:  $V = \{v_1, v_2, \dots, v_{n-1}\}$
- Lower apex vertices:  $V' = \{v'_1, v'_2, \dots, v'_{n-1}\}$

$$= \frac{(n - 1)(2n^2 + 2n - 3)}{3}$$

**Proof of (4.1.2): Degree Distance**

The degree distance of a graph  $G$  is:

$$D'(G) = \sum_{\{u,v\} \subseteq V(G)} [\deg(u) + \deg(v)] d(u, v)$$

We classify vertices by degree in  $T_n$ :

End vertices of base path:  $u_1, u_n$ , with  $\deg(u) = 2$

Internal base vertices:  $u_2, \dots, u_{n-1}$ , with  $\deg(u) = 4$

Apex vertices:  $v_1, \dots, v_{n-1}$ , with  $\deg(v) = 2$

Using the property  $D'(G) = \sum_{x \in V} \deg(x) \cdot S(x)$ ,

where  $S(x) = \sum_{y \in V} d(x, y)$

For end vertices  $u_1$  and  $u_n$ :

$$S(u_1) = S(u_n) = n(n - 1) \Rightarrow 2[S(u_1) + S(u_n)] = 4n(n - 1)$$

For internal vertices  $u_i (2 \leq i \leq n - 1)$ :

$$S(u_i) = 2i^2 - 2i(n + 1) + n^2 + n$$

For apex vertices  $v_i (1 \leq i \leq n - 1)$ :

$$S(v_i) = i(i + 1) + (n - i)(n - i + 1) - 2$$

Applying the degrees as weights:

$$D'(T_n) = 2[S(u_1) + S(u_n)] + 4 \sum_{i=2}^{n-1} S(u_i) + 2 \sum_{i=1}^{n-1} S(v_i)$$

Wiener index  $W(D(T_n))$  and the degree distance  $D'(D(T_n))$  are given by:

The total Wiener index can be computed as a sum of several components:

**1. Distances within the common path ( $W_{UU}$ )**

The vertices  $U$  form a path  $P_n$ . Using the standard formula for a path:

$$W_{UU} = \sum_{1 \leq i < j \leq n} |j - i| = \frac{n(n^2 - 1)}{6}$$

**2. Distances from path vertices to apex vertices ( $W_{UV}$  and  $W_{UV'}$ )**

The distance from a path vertex  $u_j$  to an apex vertex  $v_i$  or  $v'_i$  follows shortest path logic, same as in the single triangular snake:

$$W_{UV} + W_{UV'} = 2 \cdot \frac{n(n^2 - 1)}{3} = \frac{2n(n^2 - 1)}{3}$$

**3. Distances within apex sets ( $W_{VV}$  and  $W_{V'V'}$ )**

Each apex set (upper or lower) forms a triangular snake on its own. So:

$$W_{VV'} = \sum_{i=1}^{n-1} \sum_{j=1}^n (|j - i| + 2) = \frac{(n - 1)n(n + 1)}{3} + (n - 1)^2$$

Combine all components

$$W(D(T_n)) = W_{UU} + (W_{UV} + W_{UV'}) + (W_{VV} + W_{V'V'}) + W_{VV'} = (n - 1)(n^2 + n + 1)$$

**Proof of (4.2.2): Degree Distance**

The degree distance is defined as:

$$D'(G) = \sum_{\{u,v\} \subseteq V(G)} [\deg(u) + \deg(v)] d(u, v)$$

Classify vertices based on degree in  $D(T_n)$ :

End vertices of the path:  $u_1, u_n$ ,  $\deg(u) = 3$

Internal path vertices:  $u_2, \dots, u_{n-1}$ ,  $\deg(u) = 6$

Apex vertices (upper and lower):  $v_i, v'_i$ ,  $\deg(v) = 2$

**1. Weighted sum for end vertices**

For  $u_1$  and  $u_n$ :

$$\begin{aligned} \deg(u_1)S(u_1) + \deg(u_n)S(u_n) &= 3 \cdot S(u_1) + 3 \cdot S(u_n) \\ &= 3 \cdot 2 \cdot (n - 1)(n + 1) \\ &= 6(n - 1)(n + 1) \end{aligned}$$

**2. Weighted sum for internal path vertices**

For each  $u_i$ ,  $2 \leq i \leq n - 1$ :

$$\deg(u_i)S(u_i) = 6 \sum_{x \in V} d(u_i, x)$$

Summing over all internal path vertices accounts for distances to other path vertices and both apex sets.

**3. Weighted sum for apex vertices**

For each apex vertex  $v_i$  or  $v'_i$ :

$$\deg(v_i)S(v_i) = 2 \sum_{x \in V} d(v_i, x)$$

Combine all weighted sums

$$D'(D(T_n)) = \sum_{x \in V} \deg(x)S(x)$$

After performing the algebraic simplification and summing the arithmetic progressions:

$$W_{VV} = W_{V'V'} = \frac{(n - 1)(n - 2)(n + 3)}{6}$$

**4. Distances between upper and lower apex sets ( $W_{VV'}$ )**

For  $v_i \in V$  and  $v'_j \in V'$ , the distance is:

$$d(v_i, v'_j) = |j - i| + 2$$

Summing over all pairs:

$$D'(D(T_n)) = \frac{2(n - 1)(11n^2 + 11n - 12)}{3}$$

**Theorem 4.3:** Let  $G = T(T_n)$  be a triple triangular snake graph of order  $N = 4n - 3$  for  $n \geq 2$ . Then, the Wiener index and degree distance of  $G$  are given by:

$$W(T(T_n)) = \frac{(n - 1)(4n^2 + 4n + 15)}{3} \tag{4.3.1}$$

$$D'(T(T_n)) = 2(n - 1)(15n^2 + 15n - 16) \tag{4.3.2}$$

**Proof 4.3.1: Wiener Index  $W(T(T_n))$**

The Wiener index of a graph  $G$  is defined as:

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v)$$

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

**Step 1: Partitioning the Vertex Set**

Let the vertex set  $V$  be partitioned into:

Path vertices:  $U = \{u_1, u_2, \dots, u_n\}$

Three apex vertex sets:  $V, V', V''$ , each containing  $n - 1$  vertices

**Step 2: Distance Sums within Path and Between Path and Apex Vertices**

Distance sum within the path  $U$ :

$$\sum_{\{u_i, u_j\} \subseteq U} d(u_i, u_j) = \frac{n(n^2 - 1)}{6}$$

Distance sums between path vertices and each apex set:

$$W_{UV} = W_{UV'} = W_{UV''} = \frac{n(n^2 - 1)}{3}$$

**Step 3: Distance Sums Between Apex Sets (Inter-set)**

For vertices  $v_i \in V$  and  $v'_j \in V'$ :

$$d(v_i, v'_j) = |i - j| + 2$$

Summing over all three pairs of apex sets  $(V \times V', V \times V'', V' \times V'')$ :

$$\sum_{\text{apex pairs}} d(v_i, v_j) = 3 \sum_{i=1}^{n-1} \sum_{j=1}^{n-1} (|j - i| + 2) = 3 \cdot \frac{(n-1)(n-2)(n+3)}{6} + 3 \left( \frac{(n-1)n(n+1)}{3} + (n-1)^2 \right)$$

Combine All Contributions

$$W(T(T_n)) = \frac{n(n^2 - 1)}{6} + 3 \left( \frac{n(n^2 - 1)}{3} \right) + 3 \cdot \frac{(n-1)(n-2)(n+3)}{6} + 3 \left( \frac{(n-1)n(n+1)}{3} + (n-1)^2 \right)$$

Simplifying we get

$$W(T(T_n)) = \frac{(n-1)(4n^2 + 4n + 15)}{3}$$

**Proof 4.3.2: Degree Distance  $D'(T(T_n))$**

The degree distance of a graph  $G$  is defined as:

$$D'(G) = \sum_{\{u,v\} \in E(G)} [\deg(u) + \deg(v)] d(u, v)$$

**Step 1: Classify Vertices by Degree**

End path vertices:  $u_1, u_n$  with  $\deg(u) = 4$

Internal path vertices:  $u_i, (2 \leq i \leq n-1)$  with  $\deg(u) = 8$

Apex vertices: all  $3(n-1)$  vertices with  $\deg(v) = 2$

**Step 2: Weighted Distance Sums**

$$D'(G) = \sum_{x \in V} \deg(x) S(x)$$

where  $S(x) = \sum_{y \in V} d(x, y)$  is the sum of distances from vertex  $x$  to all other vertices.

For an endpoint  $u_1$ :

$$S(u_1) = \frac{(n-1)(4n+3)}{3}$$

For internal path vertices  $u_i$ : the contribution is weighted by  $\deg(u_i) = 8$

For apex vertices: contribution weighted by  $\deg(v) = 2$ , with total  $3(n-1)$  vertices

**Step 3: Compute Total Degree Distance**

$$D'(T(T_n)) = 2 \cdot 4S(u_1) + 8 \sum_{i=2}^{n-1} S(u_i) + 2 \sum_{j=1}^{3(n-1)} S(v_j)$$

After performing the arithmetic sum and simplifying, we get:

$$D'(T(T_n)) = 2(n-1)(15n^2 + 15n - 16)$$

**Theorem 4.4:** Let  $G = A(T_{2k})$  be an alternate triangular snake graph of order  $N = 3k$  for  $k \geq 1$ . Then, the Wiener index and degree distance of  $G$  are:

$$W(A(T_{2k})) = \frac{k(14k^2 + 9k - 5)}{6} \tag{4.4.1}$$

$$D'(A(T_{2k})) = \frac{2k(20k^2 + 9k - 11)}{3} \tag{4.4.2}$$

**Proof 4.4.1: Wiener Index  $W(A(T_{2k}))$**

The Wiener index of a graph  $G$  is:

$$W(G) = \sum_{\{u,v\} \in E(G)} d(u, v)$$

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

**Step 1: Partitioning the Vertex Set**

Let the vertex set be divided into:

Path vertices:  $U = \{u_1, u_2, \dots, u_{2k}\}$

Apex vertices:  $V_{\text{apex}} = \{v_1, v_3, \dots, v_{2k-1}\}$

**Step 2: Distance Sums within Path ( $W_{UU}$ )**

The distances between vertices on the base path  $U$  follow the standard path graph formula:

$$W_{UU} = \sum_{1 \leq i < j \leq 2k} |j - i| = \frac{2k((2k)^2 - 1)}{6} = \frac{k(4k^2 - 1)}{3}$$

**Step 3: Distance Sums Between Apex and Path Vertices ( $W_{UV}$ )**

Each apex vertex  $v_i$  is connected to  $u_i$  and  $u_{i+1}$ . The distance from  $v_i$  to a path vertex  $u_j$  is:

$$d(v_i, u_j) = \min(|i - j| + 1, |i + 1 - j| + 1)$$

Summing over all apex and path vertices:

$$W_{UV} = \sum_{i \in \{1, 3, \dots\}} \sum_{j=1}^{2k} d(v_i, u_j) = \frac{k(4k^2 + 3k - 1)}{3}$$

**Step 4: Distance Sums Between Apex Vertices ( $W_{VV}$ )**

Distance between two apex vertices  $v_i$  and  $v_j$  is:

$$d(v_i, v_j) = |j - i|$$

Summing over all pairs:

$$W_{VV} = \sum_{1 \leq i < j \leq k} 2|j - i| = \frac{k(k^2 - 1)}{3}$$

**Step 5: Combine All Contributions**

$$W(A(T_{2k})) = W_{UU} + W_{UV} + W_{VV}$$

$$= \frac{k(4k^2 - 1)}{3} + \frac{k(4k^2 + 3k - 1)}{3} + \frac{k(k^2 - 1)}{3}$$

Simplifying:

$$W(A(T_{2k})) = \frac{k(14k^2 + 9k - 5)}{6}$$

**Proof 4.4.2: Degree Distance  $D'(A(T_{2k}))$**

The degree distance of a graph  $G$  is:

$$D'(G) = \sum_{\{u,v\} \in E(G)} [\deg(u) + \deg(v)] d(u,v)$$

**Step 1: Group Vertices by Degree**

Apex vertices:  $k$  vertices with  $\deg(v) = 2$  Path endpoints:  $u_1$  and  $u_{2k}$  with  $\deg(u) = 2$

**Internal path vertices:** vertices  $u_i$  have alternating degrees 2 or 3 depending on triangular connections

**Step 2: Compute Weighted Distance Sum**

$$D'(G) = \sum_{x \in V} \deg(x) S(x)$$

where  $S(x) = \sum_{y \in V} d(x,y)$  is the sum of distances from vertex  $x$  to all others.

$$\frac{(2n-1)(2n-2)}{2} \leq \frac{(n-1)(2n^2+2n-3)}{3} \leq \frac{(2n-1)((2n-1)^2-1)}{6}$$

This verification confirms that all graphs in the investigated family, including  $D(T_n)$ ,  $T(T_n)$ , and  $A(T_n)$ , satisfy the established bounds for distance-based graph invariants.

**5.2 Corollary on Index Correlation**

We propose the following corollary concerning the relationship between the degree distance and the Wiener index for multi-layered snake graphs.

**Corollary 5.2.1:** For any graph  $G$  in the Triangular Snake family with  $n \geq 3$ , the relationship between the degree distance and the Wiener index satisfies

$$D'(G) \geq \bar{d} \cdot W(G)$$

where  $\bar{d}$  denotes the average degree of the graph.

**Proof:** By the definitions of the degree distance and the Wiener index, we have

$$D'(G) = \sum_{\{u,v\} \in E} [\deg(u) + \deg(v)] d(u,v)$$

$$W(G) = \sum_{\{u,v\} \in E} d(u,v)$$

For a graph  $G$  in which the internal vertices have a minimum degree  $k$ , we observe that

$$\deg(u) + \deg(v) \geq 2k$$

Weighted sum for apex vertices:  $2\sum S(v_i)$

Weighted sum for path vertices:  $\sum \deg(u_i) S(u_i)$

**Step 3: Combine Contributions**

Using the distance sums from Proof 6.1 and the degree weights:

$$D'(A(T_{2k})) = \frac{2k(20k^2 + 9k - 11)}{3}$$

**5. RESULTS AND DISCUSSION**

This section examines the structural properties of the derived indices and confirms their consistency with established topological bounds. The generalized expressions obtained for the Wiener index  $W(G)$  and the degree distance  $D'(G)$  for the Triangular Snake graph family are examined by comparing them with the extremal values known for connected graphs of order  $N$ .

**5.1 Verification of Universal Bounds**

According to Theorem 1 and Theorem 2, for any connected graph  $G$  of order  $N$ , the following inequalities must hold:

$$W(K_N) \leq W(G) \leq W(P_N)$$

$$D'(G) > W(G)$$

For the Triangular Snake graph  $T_n$  with order  $N = 2n - 1$ , substituting  $n$  into the derived formulas (4.1) and (4.2) gives

Let  $k_{\min}$  denote the minimum degree of any vertex in  $G$ . Then,

$$D'(G) = \sum_{\{u,v\}} [\deg(u) + \deg(v)] d(u,v)$$

$$\geq 2k_{\min} \sum_{\{u,v\}} d(u,v)$$

$$D'(G) \geq 2k_{\min} W(G)$$

For the Triple Triangular Snake graph  $T(T_n)$ , the internal path vertices have degree 8, while the apex vertices have degree 2. Consequently, the weighted summation  $D'(G)$  increases at a significantly higher rate than the Wiener index  $W(G)$ .

Substituting the specific values for the order  $N$  and size  $m$  of the graph gives

$$\frac{D'(G)}{W(G)} \approx \frac{2m}{N} = \bar{d}$$

As  $n \rightarrow \infty$ , the ratio  $\frac{D'(G)}{W(G)}$  converges to the average degree of the corresponding snake graph structure.

**5.3 Scaling of Multi-Layered Structures**

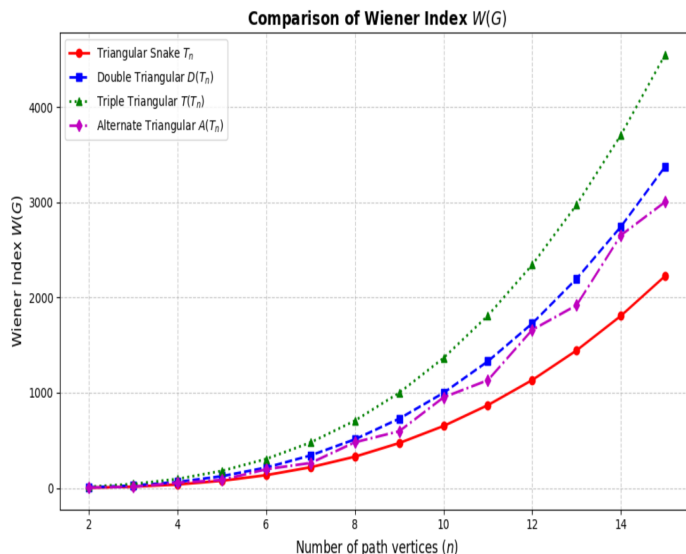
The growth of the topological indices with respect to the number of triangular layers can be summarized as follows. Linear Growth in  $N$ . The order  $N$  increases linearly:  $2n - 1 \rightarrow 3n - 2 \rightarrow 4n - 3$  corresponding to the Triangular,

Double Triangular, and Triple Triangular Snake graphs, respectively. Rapid Growth in  $D'(G)$ . Due to the increase in internal vertex degrees, the degree distance grows significantly faster than the Wiener index. In particular, for the graph  $T(T_n)$ , the degree distance is approximately three times larger than that of the basic triangular snake graph  $T_n$ .

**6. ILLUSTRATIVE ANALYSIS AND COMPARISON**

In this section, we present a graphical representation of the generalized results derived in the previous sections. The numerical values are plotted for  $2 \leq n \leq 15$  in order to observe the growth patterns and structural differences among the members of the Triangular Snake graph family.

**6.1 Growth of the Wiener Index ( $W(G)$ )**

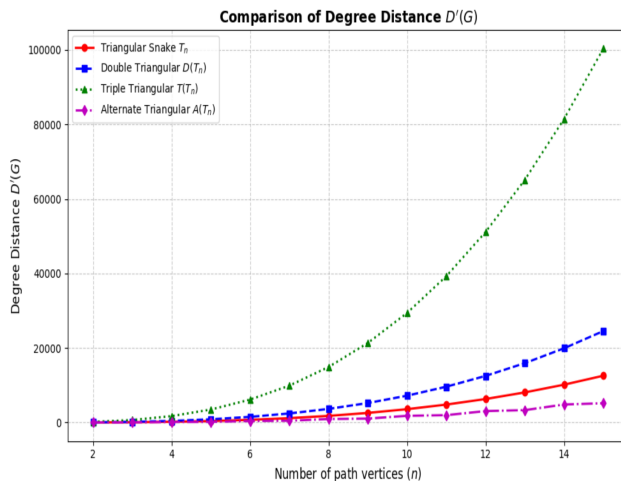


**Figure 5:** Comparative analysis of the Wiener index  $W(G)$  for the members of the Triangular Snake graph family.

As illustrated in Figure 5, the Triple Triangular Snake graph  $T(T_n)$  demonstrates the most rapid growth rate. This trend is anticipated, as  $T(T_n)$  has the largest order ( $N = 4n - 3$ ), resulting in a greater number of vertex pairs compared to  $T_n(N = 2n - 1)$  and  $A(T_n)$ . In contrast, Triangular Snake graph  $A(T_n)$  produces a curve lower than

that of  $D(T_n)$ , indicating that the structural gaps introduced in the alternating configuration effectively decrease the overall sum of distances.

**6.2 Scaling of the Degree Distance ( $D'(G)$ )**



**Figure 6:** Scaling behavior of the degree distance  $D'(G)$  for the Triangular Snake graph family.

As illustrated in Figure 6, the most notable characteristic is the sharp divergence of the curve associated with the Triple Triangular Snake graph  $T(T_n)$ . This pattern arises because the internal vertices of the central path in  $T(T_n)$  have degree 8, which greatly increases the weighted distance sums. In comparison, the Alternate Triangular Snake graph  $A(T_n)$  exhibits the lowest degree distance. This is consistent with its relatively smaller average vertex degree and the alternating arrangement of triangular attachments.

**7. APPLICATIONS IN DRUG DELIVERY NETWORK MODELING**

This section provides a mathematical perspective on the obtained distance-based indices in the context of drug delivery network modeling. Modern drug carrier systems, such as dendrimers [17, 18], polymeric scaffolds, and layered nanostructures, may be represented as finite, connected graphs  $G = (V, E)$

In this representation, vertices correspond to functional components—such as monomer units, binding regions, or active sites—while edges denote chemical linkages or diffusion routes.

Distance-based topological indices offer quantitative descriptors of structural compactness, transport efficiency, and the extent of connectivity within these networks. The closed-form expressions obtained for the Triangular Snake graph family therefore allow analytical modelling of transport-related structural properties in layered carrier architectures.

**7.1 Diffusion Efficiency via the Wiener Index**

Let drug transport within a carrier network be modelled along shortest paths between functional units. The average transport distance in a connected graph  $G$  of order  $N$  is defined as

$$\bar{d}(G) = \frac{2}{N(N-1)} W(G),$$

where

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v).$$

The quantity  $\bar{d}(G)$  represents the mean diffusion path length between all unordered vertex pairs and may be interpreted as a structural indicator of transport efficiency.

For the Triangular Snake graph  $T(T_n)$  with order  $N = 4n - 3$ , using equation (4.1.1),

$$W(T(T_n)) = \frac{(n-1)(4n^2 + 4n + 15)}{3}$$

Asymptotically,

$$W(T(T_n)) \sim \frac{4}{3}n^3, \quad \bar{d}(T(T_n)) \sim \frac{2n}{3}$$

Hence, increasing the number of triangular layers increases the average transport distance, providing a mathematical basis for diffusion scaling in multi-layered carrier structures.

**7.2 Connectivity-Weighted Transport via Degree Distance**

While the Wiener index measures pure distance effects, the Degree Distance

$$D'(G) = \sum_{\{u,v\} \subseteq V(G)} [\deg(u) + \deg(v)] d(u,v)$$

incorporates vertex connectivity into the transport model.

Define the connectivity-weighted diffusion ratio

$$\Phi(G) = \frac{D'(G)}{W(G)}$$

From corollary 5.2.1, we have

$$D'(G) \geq \bar{d}_{avg} W(G)$$

Where

$$\bar{d}_{avg} = \frac{2m}{N}$$

denotes the average degree of  $G$ .

Thus,

$$\Phi(G) \approx \bar{d}_{avg}$$

showing that the ratio between degree distance and Wiener index is governed by structural connectivity.

For the Triple Triangular Snake graph, using equation (4.3.2),

$$D'(T(T_n)) = 2(n-1)(15n^2 + 15n - 16)$$

which asymptotically satisfies

$$D'(T(T_n)) \sim 30n^3$$

Since

$$W(T(T_n)) \sim \frac{4}{3}n^3$$

we obtain

$$\Phi(T(T_n)) \sim 22.5.$$

which is significantly larger than the corresponding ratio for  $T_n$ .

This demonstrates that multi-layered triangular snake structures exhibit substantially higher connectivity-weighted transport intensity. Mathematically, increased internal vertex degrees amplify the weighted diffusion effect, leading to faster polynomial growth of  $D'(G)$  relative to  $W(G)$ . Therefore, the closed-form expressions

derived in Section 4 enable direct analytical comparison of layered network architectures under both pure distance and connectivity-weighted transport measures.

## 8. CONCLUSION

The present study provides a comprehensive mathematical analysis of distance-based topological invariants for the Triangular Snake graph family. In this work, generalized closed-form expressions for the Wiener index  $W(G)$  and the Degree Distance  $D'(G)$  were successfully derived for four distinct structural variants: the Standard Triangular Snake ( $T_n$ ), Double Triangular Snake ( $D(T_n)$ ), Triple Triangular Snake ( $T(T_n)$ ), and Alternate Triangular Snake ( $A(T_n)$ ). Through systematic algebraic derivations and graphical analysis, several important observations were obtained. First, the structural expansion resulting from the addition of triangular layers leads to cubic growth in the Wiener index. In contrast, the Degree Distance  $D'(G)$  increases at a considerably faster rate due to the higher connectivity of vertices along the central path. Furthermore, the analysis shows that the Triple Triangular Snake ( $T(T_n)$ ) produces the largest values of the investigated indices, as the maximum vertex degree reaches  $deg(u) = 8$ . On the other hand, the Alternate Triangular Snake ( $A(T_n)$ ) exhibits a more dispersed distance structure due to its alternating triangular attachments, resulting in comparatively lower index values. Additionally, all derived formulas were verified against the universal topological bounds  $W(K_n) \leq W(G) \leq W(P_n)$ , confirming the mathematical validity and consistency of the results for all  $n \geq 2$ .

In addition to the structural analysis, the derived expressions were further interpreted in terms of diffusion efficiency and connectivity-weighted transport measures. By defining the average transport distance  $\bar{d}(G) = \frac{2W(G)}{N(N-1)}$  and the connectivity ratio  $\Phi(G) = \frac{D'(G)}{W(G)}$ , it was shown that multi-layered triangular snake graphs exhibit predictable linear scaling in mean diffusion distance and accelerated polynomial growth in weighted transport intensity. These findings establish an analytical framework for comparing layered network architectures under transport-dominated processes [19].

Overall, these results enhance the understanding of structural dynamics within graph-theoretic representations of layered networks and firmly link branching intensity with diffusion behavior. The analytical approach introduced in this work extends traditional distance-based metrics while offering a scalable mathematical framework suitable for structured drug delivery systems and other processes governed by diffusion mechanisms.

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