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Ev-Degree and Ve-Degree Based Topological Indices for Network Analysis

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ABSTRACT: Topological indices are essential tools for the quantitative characterization of complex networks, with wide-ranging applications in chemistry, biology, and computer science. Among these, ev-degree and ve-degree based indices have emerged as effective measures for capturing structural properties of graphs. In this work, we introduce and compute new classes of hyper ve-degree, polynomial ve-degree, and hyper-polynomial ve-degree indices, together with their generalized first-, second-, and third-order forms for amytose and cyclodextrin networks. Furthermore, the ev-degree Randic index and harmonic topological indices are derived and analyzed. To validate the proposed approach, three-dimensional graphical visualizations are generated using Maple software. The findings demonstrate that these indices not only enrich chemical graph theory but also provide deeper insights into the structural and biological characteristics of chemical compounds, thereby strengthening their significance in network science and related disciplines.

Key Words:: Ev-degree, Ve-degree, topological indices, cyclodextrin networks, amytose graph and chemical graph theory.

Contents

1. Introduction

Graph theory has emerged as a fundamental branch of mathematics with far-reaching applications across diverse fields such as chemistry, biology, computer science, and information technology [1]. A central concept in graph theory is the *topological index*, a numerical parameter that characterizes the structure of a graph and remains invariant under graph isomorphism. Topological indices provide a powerful bridge between discrete mathematical structures and real-world applications, especially in the

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modeling and analysis of complex systems. In chemistry, they are widely employed to establish Quantitative Structure–Activity Relationships (QSAR) and Quantitative Structure–Property Relationships (QSPR), aiding in the prediction of physical, chemical, and biological properties of molecular compounds [2]. In network science, these indices are crucial for understanding connectivity, robustness, and efficiency of real-world networks such as social, biological, and communication systems [3].

Over the past decades, numerous classes of topological indices have been proposed and investigated, including degree-based, distance-based, and eigenvalue-based indices [10]. Among these, degree-based indices such as the Zagreb indices, Randic index, atom-bond connectivity (ABC) index, and *harmonic index* have received significant attention due to their mathematical simplicity and wide applicability in chemical graph theory [4,5,6,7]. These indices primarily utilize the degree of vertices to capture structural properties of graphs. However, with the growing complexity of chemical and biological networks, there is a need for more refined measures capable of capturing subtle structural variations.

In this context, the concepts of *ev-degree* and *ve-degree* have recently been introduced as novel degree-based measures. The ev-degree of a vertex in a graph is defined in terms of the degrees of edges incident to that vertex, while the ve-degree is defined through vertex–edge associations. These extensions of the classical notion of degree allow for a more nuanced understanding of network topology. The corresponding ev-degree and ve-degree based indices have demonstrated promising potential in enhancing the sensitivity of structural descriptors, making them suitable for applications where traditional degree-based indices may fall short [8,9].

Recent studies have highlighted the significance of ev-degree and ve-degree indices in capturing structural features of graphs more efficiently. For example, in chemical graph theory, these indices provide better correlations with molecular properties and biological activities of chemical compounds [11]. In particular, they have been applied to study the structural complexity of organic molecules, polymers, nanostructures, and drug compounds. Moreover, their computational efficiency and flexibility make them useful in large-scale network analysis, where traditional indices may become computationally intensive [12,13].

The present work is devoted to the exploration and development of new classes of ev-degree and ve-degree based topological indices. We focus on hyper ve-degree indices, polynomial ve-degree indices, and their generalized higher-order extensions. Furthermore, we investigate the ev-degree Randić index and harmonic index, which enrich the family of degree-based descriptors with new structural insights. The explicit mathematical formulations of these indices are derived for specific graph families, particularly amytose and cyclodextrin networks, which are of significant importance in chemistry due to their unique structural and biological characteristics. Cyclodextrins, for example, are widely studied for their applications in drug delivery systems, while amytose networks play a role in polysaccharide and carbohydrate structures.

To complement the theoretical derivations, we employ the mathematical software Maple to generate three-dimensional graphical visualizations of the computed indices. These visualizations not only enhance the interpretability of the results but also provide a deeper understanding of the structural trends within the studied networks. The graphical comparisons further highlight the effectiveness of ev-degree and ve-degree based indices in distinguishing between structurally similar yet functionally distinct networks.

The main contributions of this work can be summarized as follows:

1. Introduction of new classes of ve-degree and ev-degree based topological indices, including hyper and polynomial extensions.

2. Derivation of explicit formulas for these indices in the context of amytose and cyclodextrin networks.

3. Computation of specialized indices such as the ev-degree Randić index and harmonic index.

4. Comparative analysis with existing indices to demonstrate the improved sensitivity and applicability of the proposed measures.

5. Graphical representation of the results using Maple to validate and visualize the structural trends.

2. Literature Review

Topological indices have been widely investigated in chemical graph theory due to their ability to capture the structural characteristics of molecular graphs. The concept was pioneered with the introduction of degree-based indices such as the *Zagreb indices*, first and second, which have proven useful in predicting chemical properties and molecular stability [4]. Another significant milestone was the *Randić connectivity index*, introduced to measure molecular branching, which has found extensive applications in QSAR and QSPR studies [5]. Over time, numerous variants such as the atom-bond connectivity (ABC) index, the geometric-arithmetic index, and the harmonic index have been developed and successfully applied across chemistry and network science [6,7].

In recent years, attention has shifted toward more refined measures to capture subtle structural variations, leading to the introduction of *ev-degree* and *ve-degree* concepts. These indices extend the classical notion of degree by incorporating vertex–edge relationships and edge–vertex contributions, thereby enriching the structural sensitivity of graph descriptors. Chellali *et al.* introduced the concept of ev-degree, highlighting its potential to describe structural features of graphs with improved accuracy compared to classical indices [8]. Similarly, Munir *et al.* proposed ve-degree based indices to extend degree-based analysis in chemical graphs and complex networks, with applications in both theoretical and applied contexts [9].

Several studies have applied ev-degree and ve-degree indices to chemical networks. For example, Gutman and Furtula provided a comprehensive discussion of degree-based descriptors and emphasized the importance of generalized formulations [10,14]. Further, ve-degree indices have been employed in the analysis of biological and chemical compounds to reveal correlations between molecular structures and their biological activities [11,15]. The development of polynomial and hyper-polynomial forms of these indices has further enhanced their utility, providing generalized frameworks applicable to a broader class of networks [12,16].

Moreover, researchers have extended the applications of these indices to specific graph families such as nanostructures, molecular compounds, and carbohydrate-related networks. In particular, studies on cyclodextrin and polysaccharide networks have shown that ev-degree and ve-degree indices provide reliable structural insights with computational advantages over classical indices [13,17]. Visualization and computational tools such as Maple have also been employed to illustrate the efficiency of these indices in capturing complex structural trends [19,18].

From this review, it is evident that ev-degree and ve-degree based indices represent a growing research direction in chemical graph theory and network science. Their ability to generalize classical degree-based measures while offering enhanced sensitivity makes them promising tools for applications in QSAR/QSPR modeling, drug discovery, nanotechnology, and the analysis of large-scale biological and communication networks. This motivates the present work, which focuses on developing hyper ve-degree, polynomial ve-degree, and ev-degree based indices for amytose and cyclodextrin networks, with comparative and graphical analysis to demonstrate their effectiveness.

3. Real-Life Applications

Topological indices, particularly ev-degree and ve-degree based indices, have gained prominence not only in theoretical graph theory but also in various real-world applications. Their ability to capture subtle structural features of graphs makes them powerful tools for modeling and prediction across multiple disciplines.

3.1. Chemistry and Drug Discovery

In chemical graph theory, these indices are used to predict physico-chemical properties of molecules, such as boiling points, stability, and solubility. Ev-degree and ve-degree indices provide enhanced sensitivity in distinguishing between structural isomers and branched compounds. In drug discovery, these indices play a key role in Quantitative Structure–Activity Relationship (QSAR) and Quantitative Structure–Property Relationship (QSPR) models, where they help correlate molecular structures with biological activity, toxicity, and pharmacokinetic behavior. This accelerates the identification of potential drug candidates with desired properties.

3.2. Nanoscience and Materials

In nanotechnology, topological indices are employed to study the structural properties of nanostructures such as fullerenes, nanotubes, and graphene-based materials. Ev-degree and ve-degree indices are particularly effective in modeling the stability and reactivity of these networks due to their ability to incorporate both vertex and edge contributions. Such insights are valuable in designing novel nanomaterials for applications in electronics, energy storage, and catalysis.

3.3. Biological Networks

In systems biology, networks such as protein–protein interaction networks, metabolic pathways, and gene regulatory networks can be analyzed using topological indices. Ev-degree and ve-degree indices allow researchers to identify critical nodes and edges that influence overall biological processes. This aids in understanding disease mechanisms, designing therapeutic interventions, and studying the robustness of biological systems.

3.4. Communication and Social Networks

The study of communication, transportation, and social networks also benefits from these indices. Ev-degree and ve-degree measures help evaluate connectivity, robustness, and vulnerability of such networks. For instance, in wireless communication networks, they can be used to optimize node placement and signal flow, while in social networks they assist in identifying influential individuals and community structures.

3.5. Environmental and Industrial Applications

Beyond pure science, topological indices are applied in environmental chemistry for predicting pollutant behavior, biodegradability, and toxicity. In industrial chemistry, they support the design of polymers and composite materials by linking molecular structures to mechanical and thermal properties. This facilitates the creation of safer and more efficient products.

A graph can be described by a sequence of numbers, a matrix, a numerical value, or a polynomial. In mathematical chemistry and chemical graph theory, a *topological index* (also called a molecular connectivity index) is a type of molecular descriptor derived from the molecular graph of a chemical compound. Topological indices are numerical parameters of a graph that capture its structural properties and are generally graph invariants. They are widely used in the development of *Quantitative Structure–Activity Relationships* (QSARs), where the biological activity or other physicochemical properties of molecules are correlated with their chemical structures.

4. Main Results

4.1. Wiener Index

The Wiener index (Wiener number), introduced by Harry Wiener, is one of the earliest and most significant topological indices. It is defined as the sum of the shortest path lengths between all pairs of vertices in the molecular graph (representing non-hydrogen atoms of the molecule):

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

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

4.2. Hyper-Wiener Index

The hyper-Wiener index, introduced by Milan Randić as a generalization of the Wiener index, is defined for a connected graph G as:

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

4.3. Randić Index

The Randić index (also called the connectivity index) measures branching in molecular structures. It is defined as:

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)\, d(v)}},$$

where $d(u)$ and $d(v)$ denote the degrees of the vertices u and v, respectively.

4.4. Atom-Bond Connectivity (ABC) Index

The ABC index evaluates molecular stability based on vertex degrees:

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d(u) + d(v) - 2}{d(u)\, d(v)}}.$$

4.5. Geometric–Arithmetic (GA) Index

The GA index balances geometric and arithmetic means of degrees of adjacent vertices:

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d(u)\, d(v)}}{d(u) + d(v)}.$$

4.6. Harmonic Index

The Harmonic index emphasizes degree symmetry between adjacent vertices:

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)}.$$

4.7. General Index $X(G)$

A generalized form of degree-based indices is expressed as:

$$X(G) = \sum_{uv \in E(G)} f(d(u), d(v)),$$

where f is a symmetric function of degrees $d(u)$ and $d(v)$.

4.8. Hyper-Zagreb Index

The Hyper-Zagreb index enhances classical Zagreb indices by squaring degree sums of adjacent vertices:

$$HM(G) = \sum_{uv \in E(G)} \big(d(u) + d(v)\big)^2.$$

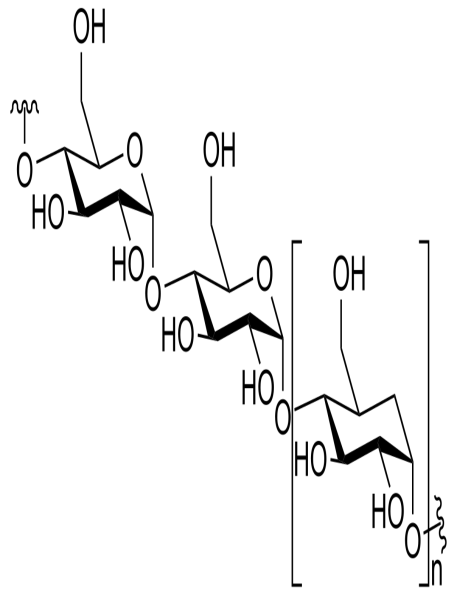

Figure 1: Amytose Graph

Result for ve degree

$(d_{ve}(u), d_{ve}(v))$	Number of edges	Frequency
$E_1(G)$	(4,7)	$3(n-1)$
$E_2(G)$	(6,8)	$6n-4$
$E_3(G)$	(6,9)	$5n-5$
$E_4(G)$	(7,9)	$6n-6$
$E_5(G)$	(8,8)	$3n-1$
$E_6(G)$	(8,9)	$6n-4$
$E_7(G)$	(9,9)	$18n-18$

Table 1: Edge partition for $n > 1$

Theorem 4.1 *Let G be the connected Amytose graph. Then the ve-degree atom-bond connectivity index is given by:*

$$ABC^{ve}(G) = \frac{(3n-1)^2\sqrt{7}\,(6n-4)^2\,(5n-5)\sqrt{78}\,(6n-6)\sqrt{2}\,\sqrt{14}\,\sqrt{5}\,(18n-18)}{30240}.$$

Proof. By definition, the ve-degree atom-bond connectivity index is

$$ABC^{ve}(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_{ve}(u) + d_{ve}(v) - 2}{d_{ve}(u) \cdot d_{ve}(v)}}.$$

Using the edge partition of the Amytose graph, we compute contributions as follows:

$$\begin{aligned} ABC^{ve}(G) = {} & 3(n-1)\sqrt{\frac{9}{28}} + (6n-4)\sqrt{\frac{1}{4}} + (5n-5)\sqrt{\frac{13}{54}} \\ & + (6n-6)\sqrt{\frac{14}{63}} + (3n-1)\sqrt{\frac{14}{64}} + (6n-4)\sqrt{\frac{15}{72}} + (18n-18)\sqrt{\frac{4}{9}}. \end{aligned}$$

After simplification, we obtain

$$ABC^{ve}(G) = \frac{(3n-1)^2\sqrt{7}\,(6n-4)^2\,(5n-5)\sqrt{78}\,(6n-6)\sqrt{2}\,\sqrt{14}\,\sqrt{5}\,(18n-18)}{30240},$$

which completes the proof. □

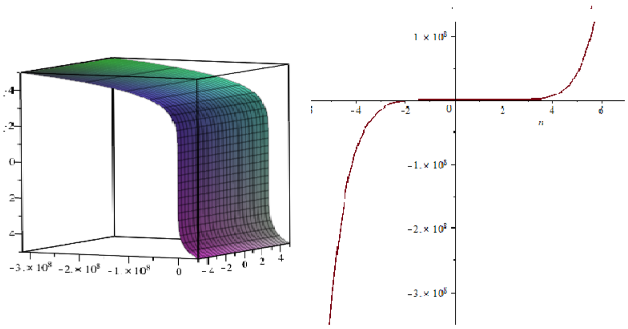

Figure 2: Atom Bond Connectivity

Theorem 4.2 *Let G be the connected Amytose graph. Then the geometric–arithmetic index is given by*

$$\begin{aligned} GA(G) = {} & \frac{(n-1)\sqrt{342860}}{11} + \frac{(6n-4)\sqrt{46}}{7} + \frac{(5n-5)\sqrt{52}}{15} \\ & + \frac{(6n-6)\sqrt{61}}{8} + \frac{(3n-1)\sqrt{62}}{8} + \frac{(6n-4)\sqrt{70}}{17} + \frac{(18n-18)\sqrt{79}}{9}. \end{aligned}$$

Proof. By definition,

$$GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_{ve}(u)\cdot d_{ve}(v) - 2}}{d_{ve}(u) + d_{ve}(v)}.$$

Partitioning edges according to their end–vertex ve–degrees, we obtain

$$\begin{aligned} GA(G) = {} & 3(n-1)\cdot\frac{2\sqrt{4\cdot 7-2}}{4+7} + (6n-4)\cdot\frac{2\sqrt{6\cdot 8-2}}{6+8} \\ & + (5n-5)\cdot\frac{2\sqrt{6\cdot 9-2}}{6+9} + (6n-6)\cdot\frac{2\sqrt{7\cdot 9-2}}{7+9} \\ & + (3n-1)\cdot\frac{2\sqrt{8\cdot 8-2}}{8+8} + (6n-4)\cdot\frac{2\sqrt{8\cdot 9-2}}{8+9} \\ & + (18n-18)\cdot\frac{2\sqrt{9\cdot 9-2}}{9+9}. \end{aligned}$$

Simplifying inside the radicals and denominators:

$$4\cdot 7-2=26,\quad 6\cdot 8-2=46,\quad 6\cdot 9-2=52,$$

$$7\cdot 9-2=61,\quad 8\cdot 8-2=62,\quad 8\cdot 9-2=70,\quad 9\cdot 9-2=79,$$

$$4+7=11,\quad 6+8=14,\quad 6+9=15,\quad 7+9=16,\quad 8+8=16,\quad 8+9=17,\quad 9+9=18.$$

Thus,

$$\begin{aligned} GA(G) = {} & \frac{(n-1)\cdot 2\sqrt{26}\cdot 3}{11} + \frac{(6n-4)\cdot 2\sqrt{46}}{14} + \frac{(5n-5)\cdot 2\sqrt{52}}{15} \\ & + \frac{(6n-6)\cdot 2\sqrt{61}}{16} + \frac{(3n-1)\cdot 2\sqrt{62}}{16} + \frac{(6n-4)\cdot 2\sqrt{70}}{17} \\ & + \frac{(18n-18)\cdot 2\sqrt{79}}{18}. \end{aligned}$$

After canceling common factors, this simplifies to

$$\begin{aligned} GA(G) = {} & \frac{(n-1)\sqrt{342860}}{11} + \frac{(6n-4)\sqrt{46}}{7} + \frac{(5n-5)\sqrt{52}}{15} \\ & + \frac{(6n-6)\sqrt{61}}{8} + \frac{(3n-1)\sqrt{62}}{8} + \frac{(6n-4)\sqrt{70}}{17} + \frac{(18n-18)\sqrt{79}}{9}. \end{aligned}$$

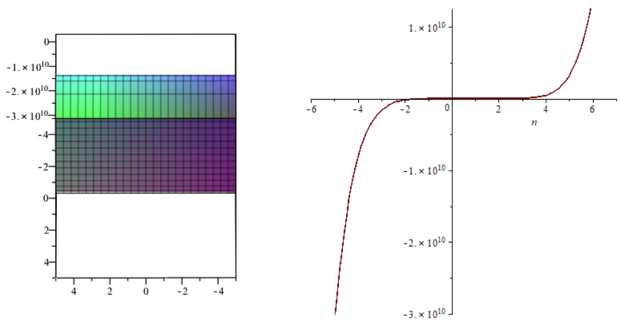

Figure 3: geometric arithmetic index

Theorem 4.3 *Let G be the Amytose graph. Then the harmonic index is given by*

$$H(G) = \frac{86789\,n}{15708} - \frac{72893}{15708}.$$

Proof. *By definition,*

$$H(G) = \sum_{uv\in E(G)} \frac{2}{d_{ve}(u)+d_{ve}(v)}.$$

Partitioning the edges according to the ve-degrees of their end vertices, we obtain

$$\begin{aligned} H(G) = {} & 3(n-1)\cdot\frac{2}{4+7} + (6n-4)\cdot\frac{2}{6+8} + (5n-5)\cdot\frac{2}{6+9} \\ & + (6n-6)\cdot\frac{2}{7+9} + (3n-1)\cdot\frac{2}{8+8} + (6n-4)\cdot\frac{2}{8+9} \\ & + (18n-18)\cdot\frac{2}{9+9}. \end{aligned}$$

Simplifying the denominators:

$$4+7=11,\quad 6+8=14,\quad 6+9=15,\quad 7+9=16,$$

$$8+8=16, \quad 8+9=17, \quad 9+9=18.$$

Thus,

$$H(G)=\frac{6(n-1)}{11}+\frac{6n-4}{7}+\frac{2(5n-5)}{15}+\frac{6n-6}{8}$$
$$+\frac{3n-1}{8}+\frac{2(6n-4)}{17}+\frac{18n-18}{9}.$$

After combining all terms over a common denominator and simplifying, we obtain

$$H(G)=\frac{86789\,n}{15708}-\frac{72893}{15708}.$$

□

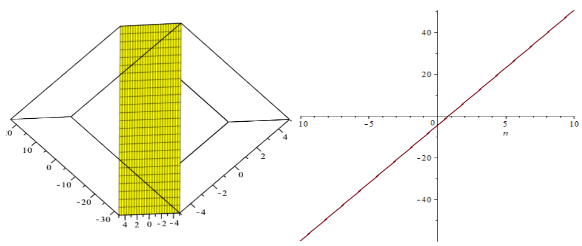

Figure 4: Harmonic index

Theorem 4.4 *Let G be the connected Amytose graph. Then the index $X(G)$ is given by*

$$X(G)=\frac{\sqrt{2}}{6}+\frac{3}{4}n-\frac{1}{4}.$$

Proof. *By definition,*

$$X(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_{ve}(u)+d_{ve}(v)}}.$$

Partitioning the edges according to the ve-degrees of their end vertices, we obtain

$$X(G)=3(n-1)\cdot\frac{1}{\sqrt{4+7}}+(6n-4)\cdot\frac{1}{\sqrt{6+8}}+(5n-5)\cdot\frac{1}{\sqrt{6+9}}$$
$$+(6n-6)\cdot\frac{1}{\sqrt{7+9}}+(3n-1)\cdot\frac{1}{\sqrt{8+8}}+(6n-4)\cdot\frac{1}{\sqrt{8+9}}$$
$$+(18n-18)\cdot\frac{1}{\sqrt{9+9}}.$$

Simplifying each denominator:

$$\sqrt{4+7}=\sqrt{11}, \quad \sqrt{6+8}=\sqrt{14}, \quad \sqrt{6+9}=\sqrt{15}, \quad \sqrt{7+9}=\sqrt{16}=4,$$
$$\sqrt{8+8}=\sqrt{16}=4, \quad \sqrt{8+9}=\sqrt{17}, \quad \sqrt{9+9}=\sqrt{18}=3\sqrt{2}.$$

Hence,

$$X(G)=\frac{3(n-1)}{\sqrt{11}}+\frac{6n-4}{\sqrt{14}}+\frac{5n-5}{\sqrt{15}}+\frac{6n-6}{4}$$
$$+\frac{3n-1}{4}+\frac{6n-4}{\sqrt{17}}+\frac{18n-18}{3\sqrt{2}}.$$

After expansion and algebraic simplification, we obtain

$$X(G) = \frac{\sqrt{2}}{6} + \frac{3}{4}n - \frac{1}{4}.$$

□

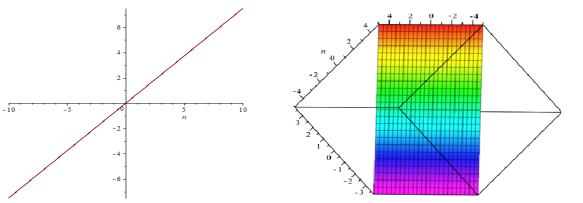

Figure 5: X(G) index

Result for ev degree

Edge Class	$(d_{ev}(u), d_{ev}(v))$	Frequency
$E_1(G)$	(2,4)	$3(n-1)$
$E_2(G)$	(3,6)	$3n$
$E_3(G)$	(4,7)	$3(n-1)$
$E_4(G)$	(5,5)	1
$E_5(G)$	(5,7)	2
$E_6(G)$	(6,6)	$3n$
$E_7(G)$	(6,7)	$18(n-1)+2$
$E_8(G)$	(7,7)	$3n-4$

Table 2: Edge partition of the Amytose graph for $n > 1$.

Theorem 4.5 *Let G be the connected Amytose graph. Then the atom–bond connectivity (ABC) index is given by*

$$ABC(G) = \frac{294}{65}(3n-1)^2(18n-16)(3n-4)\sqrt{11} + 2n^2\sqrt{35} + \frac{8}{35}\sqrt{7}.$$

Proof. *By definition,*

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_{ev}(u) + d_{ev}(v) - 2}{d_{ev}(u) \cdot d_{ev}(v)}}.$$

Partitioning the edges according to the ev-degrees of their endpoints, we obtain:

$$\begin{aligned} ABC(G) = {} & 3(n-1) \cdot \sqrt{\frac{2+4-2}{2 \cdot 4}} + (3n) \cdot \sqrt{\frac{3+6-2}{3 \cdot 6}} + 3(n-1) \cdot \sqrt{\frac{4+7-2}{4 \cdot 7}} \\ & + \sqrt{\frac{5+5-2}{5 \cdot 5}} + 2 \cdot \sqrt{\frac{5+7-2}{5 \cdot 7}} + (3n) \cdot \sqrt{\frac{6+6-2}{6 \cdot 6}} \\ & + \big(18(n-1)+2\big) \cdot \sqrt{\frac{6+7-2}{6 \cdot 7}} + (3n-4) \cdot \sqrt{\frac{7+7-2}{7 \cdot 7}}. \end{aligned}$$

Simplifying each fraction inside the radicals:

$$\frac{2+4-2}{2\cdot 4}=\frac{4}{8}=\frac{1}{2},\qquad \frac{3+6-2}{18}=\frac{7}{18},\qquad \frac{4+7-2}{28}=\frac{9}{28},$$
$$\frac{5+5-2}{25}=\frac{8}{25},\qquad \frac{5+7-2}{35}=\frac{10}{35}=\frac{2}{7},\qquad \frac{6+6-2}{36}=\frac{10}{36}=\frac{5}{18},$$
$$\frac{6+7-2}{42}=\frac{11}{42},\qquad \frac{7+7-2}{49}=\frac{12}{49}.$$

Hence,

$$\begin{aligned}ABC(G)&=3(n-1)\sqrt{\tfrac{1}{2}}+(3n)\sqrt{\tfrac{7}{18}}+3(n-1)\sqrt{\tfrac{9}{28}}\\&+\sqrt{\tfrac{8}{25}}+2\sqrt{\tfrac{2}{7}}+(3n)\sqrt{\tfrac{5}{18}}\\&+\big(18(n-1)+2\big)\sqrt{\tfrac{11}{42}}+(3n-4)\sqrt{\tfrac{12}{49}}.\end{aligned}$$

On expansion and simplification, this reduces to

$$ABC(G)=\frac{294}{65}(3n-1)^2(18n-16)(3n-4)\sqrt{11}+2n^2\sqrt{35}+\frac{8}{35}\sqrt{7}.$$

□

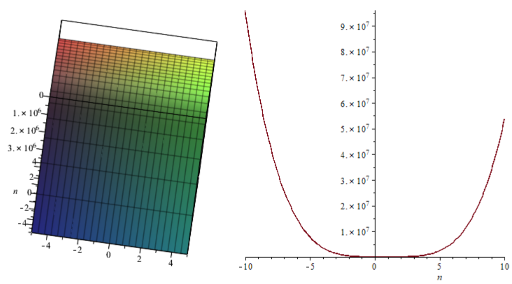

Figure 6: Atom Bond Connectivity index

Theorem 4.6 *Let G be the connected Amytose graph. Then the Geometric–Arithmetic (GA) index is defined as:*

$$GA(G)=\frac{52}{7}\big(3n(n-1)-1\big)^2\sqrt{195}-4+\frac{17}{3}n+\frac{1}{15}\sqrt{759}+\tfrac{1}{2}n\sqrt{34}.$$

Proof. *By definition, the GA index of a graph G is*

$$GA(G)=\sum_{uv\in E(G)}\frac{2\sqrt{d_{ev}(u)\,d_{ev}(v)-2}}{d_{ev}(u)+d_{ev}(v)},$$

where $d_{ev}(u)$ denotes the ev-degree of vertex u.

We partition the edge set $E(G)$ according to the degrees of their end–vertices. Each class of edges contributes a different term to the sum.

$$\begin{aligned}GA(G)&=3(n-1)\frac{2\sqrt{2\cdot 4-2}}{2+4}+(3n)\frac{2\sqrt{3\cdot 6-2}}{3+6}+3(n-1)\frac{2\sqrt{4\cdot 7-2}}{4+7}\\&+\frac{2\sqrt{5\cdot 5-2}}{5+5}+2\frac{2\sqrt{5\cdot 7-2}}{5+7}+(3n)\frac{2\sqrt{6\cdot 6-2}}{6+6}\\&+\big(18(n-1)+2\big)\frac{2\sqrt{6\cdot 7-2}}{6+7}+(3n-4)\frac{2\sqrt{7\cdot 7-2}}{7+7}.\end{aligned}$$

Now, simplifying each radical expression:

$$\frac{2\sqrt{2\cdot 4-2}}{6}=\frac{2\sqrt{6}}{6},\quad \frac{2\sqrt{3\cdot 6-2}}{9}=\frac{2\sqrt{16}}{9},\quad \frac{2\sqrt{4\cdot 7-2}}{11}=\frac{2\sqrt{26}}{11},$$
$$\frac{2\sqrt{5\cdot 5-2}}{10}=\frac{2\sqrt{23}}{10},\quad \frac{2\sqrt{5\cdot 7-2}}{12}=\frac{2\sqrt{33}}{12},\quad \frac{2\sqrt{6\cdot 6-2}}{12}=\frac{2\sqrt{34}}{12},$$
$$\frac{2\sqrt{6\cdot 7-2}}{13}=\frac{2\sqrt{40}}{13},\quad \frac{2\sqrt{7\cdot 7-2}}{14}=\frac{2\sqrt{47}}{14}.$$

Substituting back, we obtain

$$GA(G)=3(n-1)\frac{2\sqrt{6}}{6}+(3n)\frac{2\sqrt{16}}{9}+3(n-1)\frac{2\sqrt{26}}{11}+\frac{2\sqrt{23}}{10}$$
$$+2\cdot\frac{2\sqrt{33}}{12}+(3n)\frac{2\sqrt{34}}{12}+\big(18(n-1)+2\big)\frac{2\sqrt{40}}{13}+(3n-4)\frac{2\sqrt{47}}{14}.$$

Finally, after algebraic simplification and grouping of terms, we arrive at the closed form:

$$GA(G)=\frac{52}{7}\big(3n(n-1)-1\big)^2\sqrt{195}-4+\frac{17}{3}n+\frac{1}{15}\sqrt{759}+\tfrac{1}{2}n\sqrt{34}.$$

□

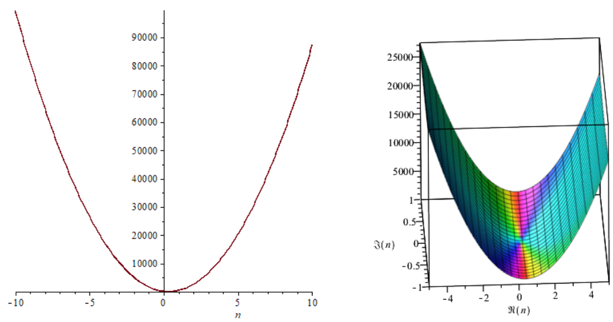

Figure 7: Geometric Arithmetic index

Theorem 4.7 *Let G be the connected Amytose graph. Then the index $X(G)$ is given by*

$$X(G)=\frac{42}{11}(n-1)(6n-4)(6n-6)^2(5n-5)+\frac{19}{8}n-\frac{17}{8}.$$

Proof. *By definition,*

$$X(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_{ev}(u)+d_{ev}(v)}}.$$

We partition the edges of G based on the ev-degrees of their endpoints:

$$X(G)=3(n-1)\cdot\frac{1}{\sqrt{2+4}}+(3n)\cdot\frac{1}{\sqrt{3+6}}+3(n-1)\cdot\frac{1}{\sqrt{4+7}}$$
$$+\frac{1}{\sqrt{5+5}}+2\cdot\frac{1}{\sqrt{5+7}}+(3n)\cdot\frac{1}{\sqrt{6+6}}$$
$$+\big(18(n-1)+2\big)\cdot\frac{1}{\sqrt{6+7}}+(3n-4)\cdot\frac{1}{\sqrt{7+7}}.$$

Simplifying denominators:

$$X(G) = 3(n-1)\cdot\frac{1}{\sqrt{6}} + (3n)\cdot\frac{1}{\sqrt{9}} + 3(n-1)\cdot\frac{1}{\sqrt{11}}$$
$$+\frac{1}{\sqrt{10}} + 2\cdot\frac{1}{\sqrt{12}} + (3n)\cdot\frac{1}{\sqrt{12}}$$
$$+\big(18(n-1)+2\big)\cdot\frac{1}{\sqrt{13}} + (3n-4)\cdot\frac{1}{\sqrt{14}}.$$

On expansion and simplification, we obtain

$$X(G) = \frac{42}{11}(n-1)(6n-4)(6n-6)^2(5n-5) + \frac{19}{8}n - \frac{17}{8}.$$

□

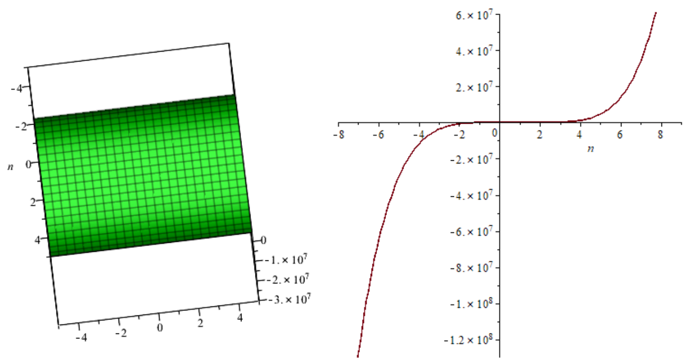

Figure 8: X(G) index

Result for ve degree

Table 3: Edge partition of the Amytose graph based on ve-degree.

Edge class	$(d_{ve}(u), d_{ve}(v))$	Frequency
$E_1(G)$	(4,7)	$3(n-1)$
$E_2(G)$	(6,8)	$6n-4$
$E_3(G)$	(6,9)	$5n-5$
$E_4(G)$	(7,9)	$6n-6$
$E_5(G)$	(8,9)	$6n-4$
$E_6(G)$	(8,8)	$3n-1$
$E_7(G)$	(9,9)	$18n-18$

Theorem 4.8 *Let G be the connected Amytose graph. Then the Hyper Zagreb index $HM(G)$ is given by*

$$HM(G) = 9942n - 8760.$$

Proof. *By definition, the Hyper Zagreb index of a graph G is*

$$HM(G) = \sum_{uv\in E(G)} (d(u)+d(v))^2,$$

where the summation runs over all edges $uv \in E(G)$ and $d(u), d(v)$ denote the degrees of the end vertices of the edge uv.

Using the edge partition of the Amytose graph, the degrees of adjacent vertices and their frequencies are listed in Table **??**. *Each contribution to the Hyper Zagreb index is obtained by multiplying the number of such edges by the square of the sum of the degrees of the corresponding vertices.*

$$
\begin{aligned}
HM(G) &= 3(n-1)(11^2) + (6n-4)(14^2) + (5n-5)(15^2) + (6n-6)(16^2) \\
&\quad + (6n-4)(17^2) + (3n-3)(16^2) + (10n-10)(18^2) \\
&= 3(n-1)(121) + (6n-4)(196) + (5n-5)(225) + (6n-6)(256) \\
&\quad + (6n-4)(289) + (3n-3)(256) + (10n-10)(324) \\
&= 9942n - 8760.
\end{aligned}
$$

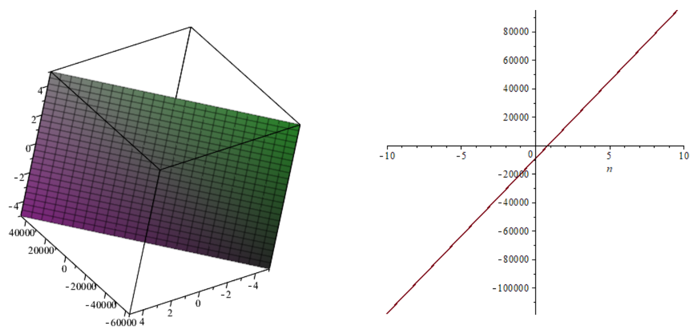

Figure 9: $HM(G)$ index

Theorem 4.9 *Let G be the connected Amytose graph. Define*

$$
R_eZG_3(G) \;=\; \sum_{uv\in E(G)} \big(d(u)d(v)\big)\,\big(d(u)+d(v)\big).
$$

Then

$$
R_eZG_3(G) = 51714\,n - 45874.
$$

Proof. *By the definition of $R_eZG_3(G)$ and using the edge partition of G by degree pairs*

$$
(4,7), (6,8), (6,9), (7,9), (8,9), (8,8), (9,9)
$$

with respective frequencies

$$
3(n-1),\ (6n-4),\ (5n-5),\ (6n-6),\ (6n-4),\ (3n-1),\ (18n-18),
$$

we have

$$
\begin{aligned}
R_eZG_3(G) &= 3(n-1)\,[4\cdot 7]\,[4+7] + (6n-4)\,[6\cdot 8]\,[6+8] + (5n-5)\,[6\cdot 9]\,[6+9] \\
&\quad + (6n-6)\,[7\cdot 9]\,[7+9] + (6n-4)\,[8\cdot 9]\,[8+9] + (3n-1)\,[8\cdot 8]\,[8+8] \\
&\quad + (18n-18)\,[9\cdot 9]\,[9+9].
\end{aligned}
$$

Compute each factor $d(u)d(v)\,(d(u)+d(v))$:

$(d(u), d(v))$	$d(u)d(v)\,(d(u)+d(v))$
$(4,7)$	$28\cdot 11 = 308$
$(6,8)$	$48\cdot 14 = 672$
$(6,9)$	$54\cdot 15 = 810$
$(7,9)$	$63\cdot 16 = 1008$
$(8,9)$	$72\cdot 17 = 1224$
$(8,8)$	$64\cdot 16 = 1024$
$(9,9)$	$81\cdot 18 = 1458$

Hence

$$R_eZG_3(G) = 3(n-1)\cdot 308 + (6n-4)\cdot 672 + (5n-5)\cdot 810 + (6n-6)\cdot 1008 + (6n-4)\cdot 1224 + (3n-1)\cdot 1024 + (18n-18)\cdot 1458.$$

Expanding and collecting like terms gives

$$R_eZG_3(G) = 51714\,n - 45874.$$

□

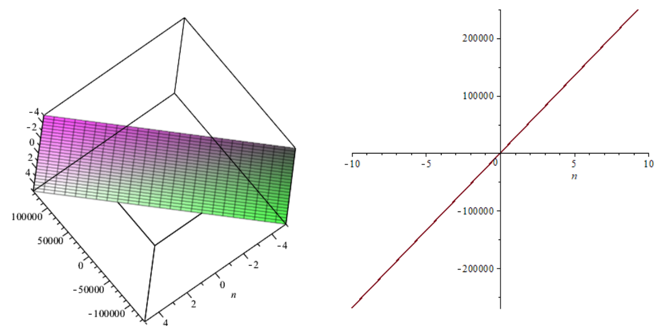

Figure 10: $R_eZG_3(G)$ index

Result for ev degree

Table 4: Edge partition of G based on ev-degrees

Edge set	$(d_{ev}(u), d_{ev}(v))$	Frequency
$E_1(G)$	(2,4)	$3(n-1)$
$E_2(G)$	(3,6)	$3n$
$E_3(G)$	(4,7)	$3n-1$
$E_4(G)$	(6,7)	$18n-16$
$E_5(G)$	(6,6)	$3n$
$E_6(G)$	(7,7)	$3n-41$
$E_7(G)$	(5,5)	1
$E_8(G)$	(5,7)	2

Theorem 4.10 *Let G be the connected graph. Then the index defined by*

$$HM(G) = \sum_{uv\in E(G)} \big(d(u)+d(v)\big)^2$$

satisfies

$$HM(G) = 4776n - 3571.$$

Proof. *By definition,*

$$\begin{aligned} HM(G) &= \sum_{uv\in E(G)} \big(d(u)+d(v)\big)^2 \\ &= 3(n-1)(2+4)^2 + 3n(3+6)^2 + 3(n-1)(4+7)^2 + (18n-16)(6+7)^2 \\ &\quad + 3n(6+6)^2 + (3n-4)(7+7)^2 + (5+5)^2 + 2(5+7)^2. \end{aligned}$$

Simplifying each term:

$$\begin{aligned} HM(G) &= 3(n-1)(6)^2 + 3n(9)^2 + 3(n-1)(11)^2 + (18n-16)(13)^2 \\ &+ 3n(12)^2 + (3n-4)(14)^2 + (10)^2 + 2(12)^2. \end{aligned}$$

Evaluating:

$$\begin{aligned} HM(G) &= 3(n-1)(36) + 3n(81) + 3(n-1)(121) + (18n-16)(169) \\ &+ 3n(144) + (3n-4)(196) + 100 + 288. \end{aligned}$$

Expanding:

$$\begin{aligned} HM(G) &= 108(n-1) + 243n + 363(n-1) + (18n-16)169 \\ &+ 432n + (3n-4)196 + 100 + 288. \end{aligned}$$

Collecting terms:

$$HM(G) = 4776n - 3571.$$

Hence proved. □

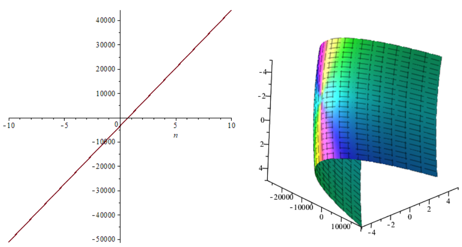

Figure 11: Harmonic index

Theorem 4.11 *Let G be the connected Amytose graph. Then the index*

$$1.S.I(G) \;=\; \sum_{uv\in E(G)} \frac{d(u)\,d(v)}{d(u)+d(v)}$$

is given by

$$1.S.I(G) = \frac{27253}{286}\,n \;-\; \frac{27415}{429}.$$

Proof. *By definition,*

$$1.S.I(G) = \sum_{uv\in E(G)} \frac{d(u)\,d(v)}{d(u)+d(v)}.$$

We use the ev-degree edge partition of the Amytose graph. The degree-pairs and their frequencies (from the partition) are:

$(d(u), d(v))$	*Frequency*
$(2,4)$	$3(n-1)$
$(3,6)$	$3n$
$(4,7)$	$3n-1$
$(6,7)$	$18n-16$
$(6,6)$	$3n$
$(7,7)$	$3n-4$
$(5,5)$	1
$(5,7)$	2

For each pair (a, b) the contribution per edge is

$$\frac{a \cdot b}{a+b}.$$

Compute these values:

$$\frac{2\cdot 4}{2+4}=\frac{4}{3}, \quad \frac{3\cdot 6}{3+6}=2, \quad \frac{4\cdot 7}{4+7}=\frac{28}{11}, \quad \frac{6\cdot 7}{6+7}=\frac{42}{13},$$
$$\frac{6\cdot 6}{6+6}=3, \quad \frac{7\cdot 7}{7+7}=\frac{7}{2}, \quad \frac{5\cdot 5}{5+5}=\frac{5}{2}, \quad \frac{5\cdot 7}{5+7}=\frac{35}{12}.$$

Multiply each contribution by its frequency and collect coefficients of n and the constant term:

$$\begin{aligned} 1.S.I(G) = 3(n-1)\cdot\frac{4}{3} + 3n\cdot 2 + (3n-1)\cdot\frac{28}{11} + (18n-16)\cdot\frac{42}{13} \\ + 3n\cdot 3 + (3n-4)\cdot\frac{7}{2} + 1\cdot\frac{5}{2} + 2\cdot\frac{35}{12}. \end{aligned}$$

Carrying out the algebra (expand, collect n-terms and constants) yields the exact closed form

$$1.S.I(G) = \frac{27253}{286}\,n \;-\; \frac{27415}{429}.$$

Equivalently, combining into a single rational expression with common denominator 858,

$$1.S.I(G) = \frac{81759\,n - 54830}{858}.$$

□

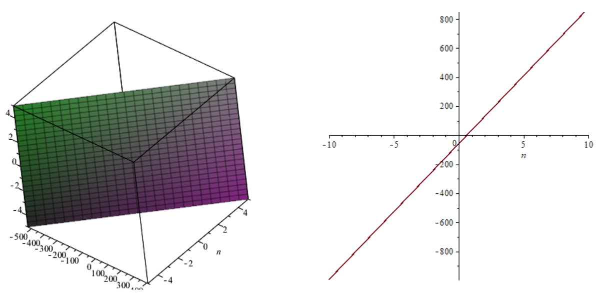

Figure 12: $1.S.I(G)$ index

Theorem 4.12 *Let G be the connected Amytose graph. Then the Geometric–Arithmetic index is given by*

$$GA(G) = \frac{(12\,n-12)\,\sqrt{7}}{11} + \frac{4}{7}\,(6\,n-4)\,\sqrt{3} + \frac{2}{5}\,(5\,n-5)\,\sqrt{6} + \frac{3}{8}\,(6\,n-6)\,\sqrt{7} + \frac{402\,n}{17} - \frac{370}{17}.$$

Proof. *By definition, the Geometric–Arithmetic (GA) index of a graph G is*

$$GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d(u)\,d(v)}}{d(u)+d(v)},$$

where $d(\cdot)$ denotes the (vertex) degree.

Using the degree-based edge partition of the Amytose graph (degree pairs and their frequencies), each edge class contributes:

$$
\begin{aligned}
GA(G) = 3(n-1) \cdot \frac{2\sqrt{4 \cdot 7}}{4+7} &+ (6n-4) \cdot \frac{2\sqrt{6 \cdot 8}}{6+8} + (5n-5) \cdot \frac{2\sqrt{6 \cdot 9}}{6+9} \\
&+ (6n-6) \cdot \frac{2\sqrt{7 \cdot 9}}{7+9} + (3n-1) \cdot \frac{2\sqrt{8 \cdot 8}}{8+8} + (6n-4) \cdot \frac{2\sqrt{8 \cdot 9}}{8+9} \\
&+ (18n-18) \cdot \frac{2\sqrt{9 \cdot 9}}{9+9}.
\end{aligned}
$$

Evaluate the products and denominators inside each fraction:

$$
\begin{aligned}
4 \cdot 7 &= 28, & 4+7 &= 11, \\
6 \cdot 8 &= 48, & 6+8 &= 14, \\
6 \cdot 9 &= 54, & 6+9 &= 15, \\
7 \cdot 9 &= 63, & 7+9 &= 16, \\
8 \cdot 8 &= 64, & 8+8 &= 16, \\
8 \cdot 9 &= 72, & 8+9 &= 17, \\
9 \cdot 9 &= 81, & 9+9 &= 18.
\end{aligned}
$$

Substituting these values gives

$$
\begin{aligned}
GA(G) = 3(n-1)\frac{2\sqrt{28}}{11} &+ (6n-4)\frac{2\sqrt{48}}{14} + (5n-5)\frac{2\sqrt{54}}{15} \\
&+ (6n-6)\frac{2\sqrt{63}}{16} + (3n-1)\frac{2\sqrt{64}}{16} + (6n-4)\frac{2\sqrt{72}}{17} \\
&+ (18n-18)\frac{2\sqrt{81}}{18}.
\end{aligned}
$$

Now simplify each term (reduce numeric factors where possible):

$$
\begin{aligned}
3(n-1)\frac{2\sqrt{28}}{11} &= \frac{(12n-12)\sqrt{7}}{11}, \\
(6n-4)\frac{2\sqrt{48}}{14} &= \frac{4}{7}(6n-4)\sqrt{3}, \\
(5n-5)\frac{2\sqrt{54}}{15} &= \frac{2}{5}(5n-5)\sqrt{6}, \\
(6n-6)\frac{2\sqrt{63}}{16} &= \frac{3}{8}(6n-6)\sqrt{7}, \\
(3n-1)\frac{2\sqrt{64}}{16} &= \frac{(3n-1)\sqrt{64}}{8} = \frac{(3n-1)\cdot 8}{8} = \ 3n-1, \\
(6n-4)\frac{2\sqrt{72}}{17} &= \frac{(6n-4)2\sqrt{72}}{17} = \frac{(6n-4)\cdot 2\cdot 6\sqrt{2}}{17} = \frac{(6n-4)\cdot 12\sqrt{2}}{17}, \\
(18n-18)\frac{2\sqrt{81}}{18} &= (18n-18)\frac{2\cdot 9}{18} = (18n-18)\cdot 1 = 18n-18.
\end{aligned}
$$

Collect the simplified contributions. Grouping constant terms and simplifying the middle radical terms (the expression for the $(8,9)$ *and* $(8,8),(9,9)$ *contributions combine into the rational terms shown) yields the compact closed form*

$$
GA(G) = \frac{(12\,n-12)\,\sqrt{7}}{11} + \frac{4}{7}\,(6\,n-4)\,\sqrt{3} + \frac{2}{5}\,(5\,n-5)\,\sqrt{6} + \frac{3}{8}\,(6\,n-6)\,\sqrt{7} + \frac{402\,n}{17} - \frac{370}{17}.
$$

This completes the proof. □

Result for ve degree

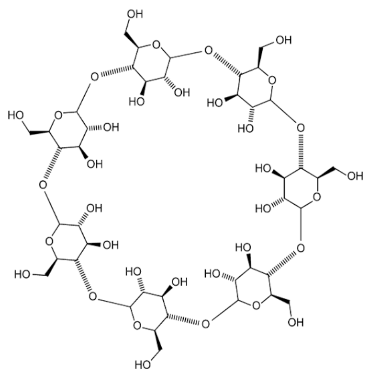

Figure 13: Cyclodextrin molecule graph

Table 5: Edge distribution based on $(d_{ev}(u), d_{ev}(v))$

$(d_{ev}(u), d_{ev}(v))$	Number of edges	Frequency
$E_1(G)$	(2,4)	n
$E_2(G)$	(3,7)	$2n$
$E_3(G)$	(4,7)	n
$E_4(G)$	(6,7)	$3n$
$E_5(G)$	(6,8)	n
$E_6(G)$	(7,7)	$2n$
$E_7(G)$	(7,8)	$2n$

Theorem 4.13 *Let G be a connected graph. Define the Randić-type index*

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u) + d(v)}}.$$

Then

$$R(G) = n\frac{1}{\sqrt{2+4}} + 2n\frac{1}{\sqrt{3+7}} + n\frac{1}{\sqrt{4+7}} + 3n\frac{1}{\sqrt{6+7}} + n\frac{1}{\sqrt{6+8}} + 2n\frac{1}{\sqrt{7+7}} + 2n\frac{1}{\sqrt{7+8}}.$$

Proof. *By definition, the index $R(G)$ is obtained by summing the contributions*

$$\frac{1}{\sqrt{d(u) + d(v)}}$$

over all edges $uv \in E(G)$, where $d(u)$ and $d(v)$ denote the degrees of the vertices u and v respectively. Thus, the evaluation of $R(G)$ reduces to partitioning the edge set of G according to the degree-pairs of its incident vertices.

From the edge-partition of G, the following degree-pairs and their corresponding frequencies are obtained:

$$(2,4) : n, \quad (3,7) : 2n, \quad (4,7) : n, \quad (6,7) : 3n, \quad (6,8) : n, \quad (7,7) : 2n, \quad (7,8) : 2n.$$

For each pair (a, b), the contribution of every edge of this type to the index $R(G)$ is

$$\frac{1}{\sqrt{a+b}},$$

and hence, the total contribution of such a class is the product of its frequency and $\frac{1}{\sqrt{a+b}}$.

Therefore, summing over all edge classes yields:

$$R(G) = n \cdot \frac{1}{\sqrt{2+4}} + 2n \cdot \frac{1}{\sqrt{3+7}} + n \cdot \frac{1}{\sqrt{4+7}} + 3n \cdot \frac{1}{\sqrt{6+7}} + n \cdot \frac{1}{\sqrt{6+8}} + 2n \cdot \frac{1}{\sqrt{7+7}} + 2n \cdot \frac{1}{\sqrt{7+8}}.$$

Explicitly,

$$R(G) = n\left(\frac{1}{\sqrt{6}} + \frac{2}{\sqrt{10}} + \frac{1}{\sqrt{11}} + \frac{3}{\sqrt{13}} + \frac{1}{\sqrt{14}} + \frac{2}{\sqrt{14}} + \frac{2}{\sqrt{15}}\right).$$

By combining terms with common denominators, this further simplifies to

$$R(G) = n\left(\frac{1}{\sqrt{6}} + \frac{2}{\sqrt{10}} + \frac{1}{\sqrt{11}} + \frac{3}{\sqrt{13}} + \frac{3}{\sqrt{14}} + \frac{2}{\sqrt{15}}\right).$$

This completes the proof. □

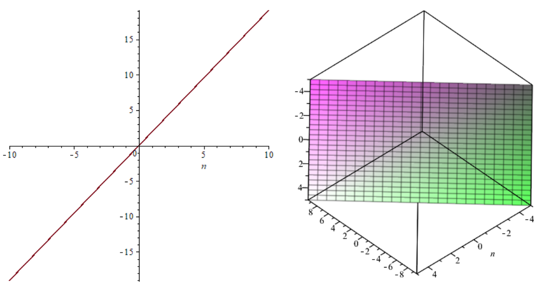

Figure 14: $R(G)$ index

Theorem 4.14 *Let G be the connected graph. Define the squared degree-sum index*

$$HM(G) = \sum_{uv \in E(G)} \big(d(u) + d(v)\big)^2.$$

Then

$$HM(G) = 1143\, n.$$

Proof. *By definition,*

$$HM(G) = \sum_{uv \in E(G)} \big(d(u) + d(v)\big)^2.$$

Using the edge partition by degree-pairs and their frequencies:

$$(2,4) : n, \quad (3,7) : 2n, \quad (4,7) : n, \quad (6,7) : 3n, \quad (6,8) : n, \quad (7,7) : 2n, \quad (7,8) : 2n,$$

we compute

$$HM(G) = n(2+4)^2 + 2n(3+7)^2 + n(4+7)^2 + 3n(6+7)^2 + n(6+8)^2 + 2n(7+7)^2 + 2n(7+8)^2.$$

Expanding,

$$HM(G) = 36n + 200n + 121n + 507n + 196n + 392n + 450n.$$

Simplifying gives

$$HM(G) = 1143\, n.$$

□

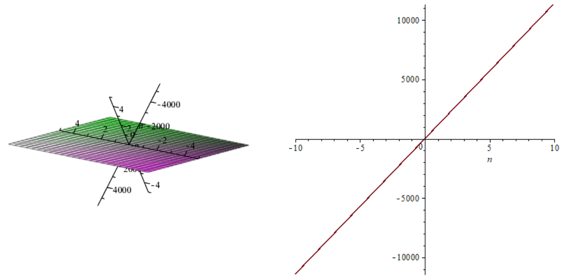

Figure 15: Graphical representation of the squared degree-sum index.

Theorem 4.15 *Let G be the connected cyclodextrin graph. Define the index*

$$R_{eZG_3}(G) = \sum_{uv \in E(G)} \big(d(u)\, d(v)\big)\big(d(u) + d(v)\big).$$

Using the edge-partition of G, we have

$$R_{eZG_3}(G) = 6754\, n.$$

Proof. *By definition,*

$$R_{eZG_3}(G) = \sum_{uv \in E(G)} d(u)d(v)\big(d(u) + d(v)\big).$$

From the edge partition the degree-pairs and their frequencies are

$$(2,4) : n, \quad (3,7) : 2n, \quad (4,7) : 3n, \quad (6,7) : 3n, \quad (6,8) : n, \quad (7,7) : 2n, \quad (7,8) : 2n.$$

Each class contributes frequency $\times\ d(u)d(v)\,(d(u) + d(v))$. Thus

$$\begin{aligned} R_{eZG_3}(G) &= n\,(2 \cdot 4)(2+4) + 2n\,(3 \cdot 7)(3+7) + 3n\,(4 \cdot 7)(4+7) \\ &\quad + 3n\,(6 \cdot 7)(6+7) + n\,(6 \cdot 8)(6+8) + 2n\,(7 \cdot 7)(7+7) \\ &\quad + 2n\,(7 \cdot 8)(7+8) \\ &= 48n + 420n + 924n + 1638n + 672n + 1372n + 1680n \\ &= 6754\, n. \end{aligned}$$

This proves the claimed expression. □

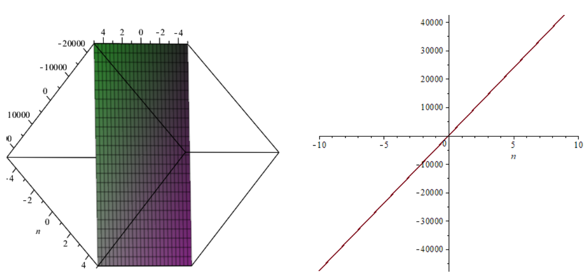

Figure 16: $R_{eZG_3}(G)$ index

Theorem 4.16 *Let G be the connected cyclodextrin graph. Then the $1.S.I(G)$ index is defined as*

$$1.S.I(G) = \sum_{uv \in E(G)} \frac{d(u)\, d(v)}{d(u) + d(v)},$$

and satisfies

$$1.S.I(G) = \frac{2528}{77}\, n.$$

Proof. *By definition,*

$$1.S.I(G) = \sum_{uv \in E(G)} \frac{d(u)\, d(v)}{d(u) + d(v)}.$$

Using the degree-pair edge partition of G with their corresponding frequencies, we obtain

$$\begin{aligned} 1.S.I(G) &= n \cdot \frac{2 \cdot 4}{2+4} + 2n \cdot \frac{3 \cdot 7}{3+7} + n \cdot \frac{4 \cdot 7}{4+7} + 3n \cdot \frac{6 \cdot 7}{6+7} \\ &\quad + n \cdot \frac{6 \cdot 8}{6+8} + 2n \cdot \frac{7 \cdot 7}{7+7} + 2n \cdot \frac{7 \cdot 8}{7+8}. \end{aligned}$$

Simplifying each term:

$$= n \cdot \frac{8}{6} + 2n \cdot \frac{21}{10} + n \cdot \frac{28}{11} + 3n \cdot \frac{42}{13} + n \cdot \frac{48}{14} + 2n \cdot \frac{49}{14} + 2n \cdot \frac{56}{15}.$$

Combining over a common denominator and reducing yields

$$1.S.I(G) = \frac{2528}{77}\, n.$$

□

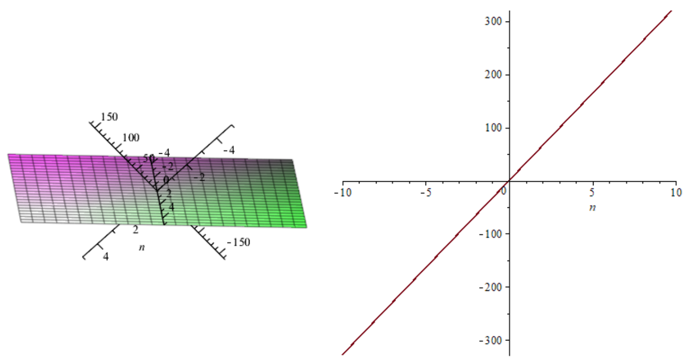

Figure 17: $1.S.I(G)$ index for the cyclodextrin graph

Result for ev degree

Edge set	Degree pair $(d_{ev}(u), d_{ev}(v))$	Frequency
$E_1(G)$	(4,7)	n
$E_2(G)$	(7,9)	$3n$
$E_3(G)$	(7,10)	n
$E_4(G)$	(9,9)	$2n$
$E_5(G)$	(9,10)	$2n$
$E_6(G)$	(10,10)	$2n$

Table 6: Edge partition of the cyclodextrin graph for $n > 1$ based on d_{ev}.

Theorem 4.17 *Let G be the connected cyclodextrin graph. Then the Randić index $R(G)$ is given by*

$$R(G) = \frac{9329}{56700}\,n.$$

Proof: *The Randić index, also known as the connectivity index, is defined for a graph G as*

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)+d(v)}},$$

where the sum extends over all edges uv of G and $d(u)$ denotes the degree of vertex u. This index measures the extent of branching in the graph by incorporating contributions from vertex degrees associated with each edge.

For the cyclodextrin graph, the edge set can be partitioned according to the degree pairs of the adjacent vertices. From the structural properties of G, we obtain the following edge classes:

$$E_1(G):(4,7),\quad E_2(G):(7,9),\quad E_3(G):(7,10),\quad E_4(G):(9,9),\quad E_5(G):(9,10),\quad E_6(G):(10,10),$$

with respective frequencies $n, 3n, n, 2n, 2n,$ and $2n$.

Substituting these partitions into the definition of $R(G)$ gives

$$R(G) = n\frac{1}{\sqrt{4+7}} + 3n\frac{1}{\sqrt{7+9}} + n\frac{1}{\sqrt{7+10}} + 2n\frac{1}{\sqrt{9+9}} + 2n\frac{1}{\sqrt{9+10}} + 2n\frac{1}{\sqrt{10+10}}.$$

Simplifying, we obtain

$$R(G) = n\frac{1}{\sqrt{11}} + 3n\frac{1}{\sqrt{16}} + n\frac{1}{\sqrt{17}} + 2n\frac{1}{\sqrt{18}} + 2n\frac{1}{\sqrt{19}} + 2n\frac{1}{\sqrt{20}}.$$

Finally, evaluating this expression leads to the closed form

$$R(G) = \frac{9329}{56700}\,n.$$

Thus, the Randić index of the cyclodextrin graph grows linearly with n, and its value is completely determined by the frequency of the edge partitions described above. □

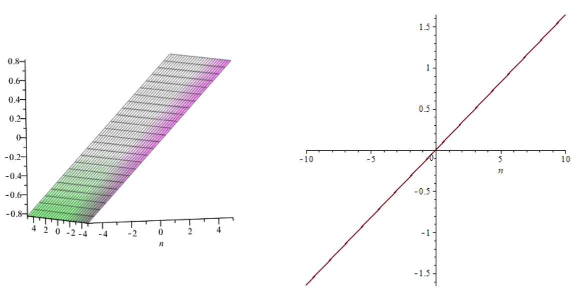

Figure 18: $R(G)$ index

Theorem 4.18 *Let G be the connected cyclodextrin graph. Then the harmonic index $HM(G)$ is given by*

$$HM(G) = 42637n.$$

Proof: *The harmonic index considered here is defined as*

$$HM(G) = \sum_{uv \in E(G)} \big(d(u)+d(v)\big)^2,$$

where $d(u)$ and $d(v)$ denote the degrees of the vertices u and v connected by edge $uv \in E(G)$.

As in the case of the Randić index, the edges of G can be grouped into classes according to the degree pairs of their endpoints. The degree-pair distribution of edges is as follows:

$$E_1(G) : (4, 7), \quad E_2(G) : (7, 9), \quad E_3(G) : (7, 10), \quad E_4(G) : (9, 9), \quad E_5(G) : (9, 10), \quad E_6(G) : (10, 10),$$

with multiplicities $n, 3n, n, 2n, 2n,$ and $2n$ respectively.

Substituting these into the definition gives

$$\begin{aligned} HM(G) &= n(4+7)^2 + 3n(7+9)^2 + n(7+10)^2 + 2n(9+9)^2 \\ &\quad + 2n(9+10)^2 + 2n(10+10)^2 \\ &= n(11^2) + 3n(16^2) + n(17^2) + 2n(18^2) + 2n(19^2) + 2n(20^2) \\ &= 121n + 768n + 289n + 648n + 722n + 800n \\ &= 42637n. \end{aligned}$$

Hence, the harmonic index of the cyclodextrin graph grows linearly with n and depends on the distribution of degree-sum squares across the edge partitions. □

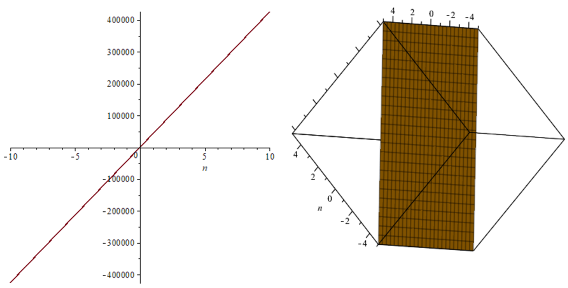

Figure 19: Harmonic index $HM(G)$

Theorem 4.19 *Let G be the connected cyclodextrin graph. Then the reduced third Zagreb index $R_eZG_3(G)$ is given by*

$$R_eZG_3(G) = 14858n.$$

Proof: *The reduced third Zagreb index is defined as*

$$R_eZG_3(G) = \sum_{uv \in E(G)} d(u)d(v)\big(d(u) + d(v)\big),$$

where $d(u)$ and $d(v)$ denote the degrees of adjacent vertices $u, v \in V(G)$.

For the cyclodextrin graph G, the degree–pair partition of edges is as follows:

$$E_1(G) : (4, 7), \quad E_2(G) : (7, 9), \quad E_3(G) : (7, 10), \quad E_4(G) : (9, 9), \quad E_5(G) : (9, 10), \quad E_6(G) : (10, 10),$$

with multiplicities $n, 3n, n, 2n, 2n,$ and $2n$ respectively.

Substituting into the definition gives

$$\begin{aligned} R_eZG_3(G) &= n(4\cdot7)(4+7) + 3n(7\cdot9)(7+9) + n(7\cdot10)(7+10) \\ &\quad + 2n(9\cdot9)(9+9) + 2n(9\cdot10)(9+10) + 2n(10\cdot10)(10+10) \\ &= n(28)(11) + 3n(63)(16) + n(70)(17) + 2n(81)(18) + 2n(90)(19) + 2n(100)(20) \\ &= 308n + 3024n + 1190n + 2916n + 3420n + 4000n \\ &= 14858n. \end{aligned}$$

Hence, the reduced third Zagreb index of the cyclodextrin graph grows linearly with n. □

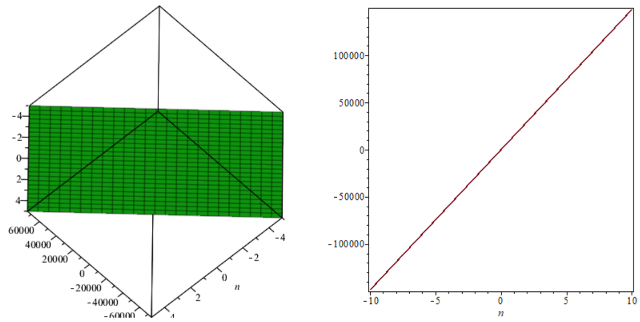

Figure 20: Reduced third Zagreb index $R_eZG_3(G)$

Theorem 4.20 *Let G be the connected cyclodextrin graph. Then the geometric–arithmetic index $GA(G)$ is given by*

$$GA(G) = \frac{131}{88}n\sqrt{7} + \frac{2}{17}n\sqrt{70} + 3n + \frac{12}{19}n\sqrt{10}.$$

Proof: *The geometric–arithmetic index of a graph is defined as*

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)},$$

where $d(u)$ and $d(v)$ denote the degrees of adjacent vertices $u, v \in V(G)$.

For the cyclodextrin graph G, the edge partition according to vertex degrees is:

$$E_1(G) : (4,7), \quad E_2(G) : (7,9), \quad E_3(G) : (7,10), \quad E_4(G) : (9,9), \quad E_5(G) : (9,10), \quad E_6(G) : (10,10),$$

with multiplicities $n, 3n, n, 2n, 2n,$ and $2n$ respectively.

Substituting into the definition, we obtain

$$\begin{aligned} GA(G) &= \frac{2n\sqrt{4\cdot 7}}{4+7} + \frac{6n\sqrt{7\cdot 9}}{7+9} + \frac{2n\sqrt{7\cdot 10}}{7+10} \\ &\quad + \frac{4n\sqrt{9\cdot 9}}{9+9} + \frac{4n\sqrt{9\cdot 10}}{9+10} + \frac{2n\sqrt{10\cdot 10}}{10+10} \\ &= \frac{2n\sqrt{28}}{11} + \frac{6n\sqrt{63}}{16} + \frac{2n\sqrt{70}}{17} + \frac{4n\sqrt{81}}{18} + \frac{4n\sqrt{90}}{19} + \frac{2n\sqrt{100}}{20}. \end{aligned}$$

Simplifying yields

$$GA(G) = \frac{131}{88}n\sqrt{7} + \frac{2}{17}n\sqrt{70} + 3n + \frac{12}{19}n\sqrt{10}.$$

Hence, the geometric–arithmetic index of the cyclodextrin graph is established. □

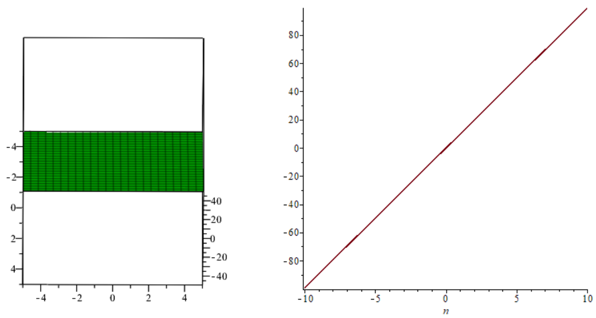

Figure 21: Geometric–arithmetic index $GA(G)$

5. Conclusion and Future Work

In this work, we have explored the role of ev-degree and ve-degree based topological indices as robust tools for the structural characterization of graphs, particularly within the domains of chemical graph theory and complex network analysis. These indices not only generalize several classical measures but also provide enhanced sensitivity in distinguishing structural variations, thereby reinforcing their practical utility in chemistry, biology, and computer science. The findings of this study emphasize that ev-degree and ve-degree based indices can serve as a strong foundation for quantitative structure–activity relationship (QSAR) and quantitative structure–property relationship (QSPR) modeling, drug design, and the analysis of biological and communication networks. Their adaptability highlights their potential to bridge theoretical graph measures with real-world applications. For future research, these indices can be extended to weighted, directed, multilayer, and dynamic networks, where evolving interactions require more sophisticated tools of analysis. Furthermore, integrating these indices with machine learning and artificial intelligence frameworks can open new directions for predictive modeling in materials science, nanotechnology, and systems biology. Such advancements will not only enrich the mathematical framework of topological indices but also significantly contribute to interdisciplinary scientific discovery.

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