mathematics

Article

Evaluation of Various Topological Indices of Flabellum Graphs

Xiaolong Shi [1], Saeed Kosari [1,*], Uzma Ahmad [2], Saira Hameed [2] and Sadia Akhter [2]

[1] Institute of Computing Science and Technology, Guangzhou University, Guangzhou 510006, China; xlshi@gzhu.edu.cn
[2] Department of Mathematics, University of the Punjab, Lahore 54590, Pakistan; uzma.math@pu.edu.pk (U.A.); saira.math@pu.edu.pk (S.H.); sadiaakhtar251@gmail.com (S.A.)
* Correspondence: saeedkosari38@gzhu.edu.cn

Abstract: Graph theory serves as an engaging arena for the investigation of proof methods within the field of discrete mathematics, and its findings find practical utility in numerous scientific domains. Chemical graph theory is a specialized branch of mathematics that uses graphs to represent and analyze the structure and properties of chemical compounds. Topological indices are mathematical properties of graphs that play a crucial role in chemistry. They provide a unique way to connect the structural characteristics of chemical compounds to their corresponding molecular graphs. The flabellum graph $F_n^{(k,j)}$ is obtained with the help of $k \geq 2$ duplicates of the cycle graph C_n with a common vertex (known as, central vertex). Then, in j of these duplicates, additional edges are added, joining the central vertex to all non-adjacent vertices. In this article, we compute different degree-based topological indices for flabellum graphs, including some well known indices, such as the Randić index, the atom bond connectivity index, the geometric–arithmetic index, and the Zagreb indices. This research provides an in-depth examination of these specific indices within the context of flabellum graphs. Moreover, the behavior of these indices is shown graphically, in terms of the parameters j, k, and n. Additionally, we have extended the concept of the first Zagreb index, to address the issue of cybercrime. This application enables us to identify criminals who exhibit higher levels of activity and engagement in multiple criminal activities when compared to their counterparts. Furthermore, we conducted a comprehensive comparative analysis of the first Zagreb index against the closeness centrality measure. This analysis sheds light on the effectiveness and relevance of the topological index in the context of cybercrime detection and network analysis.

Keywords: Zagreb index; Randić index; chemical graph theory; flabellum graphs

MSC: 05C05; 05C07; 05C12; 05C35

Citation: Shi, X.; Kosari, S.; Ahmad, U.; Hameed, S.; Akhter, S. Evaluation of Various Topological Indices of Flabellum Graphs. *Mathematics* **2023**, *11*, 4167. https://doi.org/10.3390/math11194167

Academic Editors: Hilal Ahmad and Yilun Shang

Received: 26 August 2023
Revised: 25 September 2023
Accepted: 26 September 2023
Published: 5 October 2023

1. Introduction

Consider $\mathtt{G} = (\mathtt{V}, \mathtt{E})$, a simple connected graph, having a vertex set and an edge set $\mathtt{V}$ and $\mathtt{E}$, respectively. Let the order and the size of graph be n and m, respectively. In this context, d_v is the degree of a vertex v or the count of edges that are incident to v or the number of vertices which are adjacent to v. The distance between two vertices, u and v, denoted as $d(u, v)$, is a measure of the shortest path (also known as the geodesic) between u and v within the graph $\mathtt{G}$. It is defined as the number of edges present in the shortest path connecting u and v. A molecular graph is a type of connected, undirected graph that can be uniquely associated with the structural formula of a chemical compound. In this graph, the nodes represent the atoms present in the molecule, and the edges symbolize the chemical bonds between these atoms.

To tackle organic chemistry difficulties, the chemical graph theory incorporates graph theory with chemistry [1]. The relationships between structured properties (QSPR) and structured activities (QSAR) is one of the most critical issues in this discipline [1].

Topological indices are actively used in QSPR/QSAR research [2]. Topological indices play a pivotal role in unraveling the structural intricacies that govern the properties and behaviors of molecules and networks [3]. These numerical descriptors provide valuable quantitative information about the underlying topology, enabling researchers to classify, compare, and predict various characteristics and phenomena. The study and calculation of topological indices have found wide-ranging applications in computational biology, chemistry, materials science, and network analysis [4]. Topological indices represent mathematical expressions applicable to any graph used to model molecular structures. These indices enable the analysis of mathematical parameters, facilitating the exploration of various physicochemical characteristics of a molecule. They can be used to predict the solubility of organic compounds. They help identify molecular features that affect a molecule's ability to dissolve in a solvent. Indices can provide insights into a molecule's boiling and melting points, aiding in the selection of compounds with desirable physical properties for various applications. QSAR models use topological indices to relate the chemical structure of compounds to their biological activity. This is crucial in drug discovery and design. These indices help in identifying correlations between different physicochemical properties of molecules, enabling a better understanding of molecular behavior. Consequently, these indices serve as efficient means to avoid the need for costly and time-consuming laboratory experiments.

The remarkable growth in computational power and the development of sophisticated algorithms have paved the way for the exploration and utilization of diverse topological indices. These indices offer insights into the connectivity patterns, branching characteristics, and distance relationships within molecules and graphs. By encapsulating these features into numerical representations, researchers gain a powerful tool to investigate molecular properties, design new compounds, understand biological activities, and analyze complex networks.

Among the plethora of topological indices available, several prominent ones have emerged as widely used and extensively studied descriptors. The Wiener Index [5], for instance, calculates the sum of the lengths of the shortest paths between all pairs of vertices in a molecular structure or graph, providing a measure of overall branching and connectivity. It shows the behaviors of boiling points of chemical graphs. Another renowned index is the Randić index [6], which correlates bond multiplicities with the sum of reciprocal square roots, aiding in the prediction of various physicochemical properties.

The Zagreb indices [7] capture the degrees of vertices and their pairwise interactions, shedding light on the structural diversity within a molecule or graph. Similarly, the Balaban index [8] offers a distance-based measure of non-adjacency between pairs of vertices, with implications for chemical reactivity and biological activity predictions. The Hosoya index [9], on the other hand, quantifies the number of matchings or pairs of non-adjacent vertices, revealing the size and complexity of a molecular structure.

Several properties of the sum connectivity index [10] have been investigated. These include bounding and characterizing graphs of different types, identifying extremal graphs based on sum connectivity index (or SCI). A noteworthy observation is the striking similarity in correlation properties between the product connectivity index and the sum connectivity index. The graph represented by the notation $D_n^{(k)}$ is known as the Dutch windmill graph, and it is constructed with the help of k duplicates of C_n (the cycle graph) while sharing a common vertex among them. Considerable research has already been conducted on topological indices for Dutch windmill graphs. Various studies have explored the structural and mathematical properties of these graphs and their correlation with topological indices. Researchers have investigated the Wiener index, the Randić index, the Zagreb indices, and other topological measures, to better understand the characteristics and complexity of Dutch windmill graphs [11].

In [12], the authors outlined the fundamental uses of distance-based entropy in the realm of chemistry, which encompass signal processing, investigations into crystal structures, analysis of molecular ensembles, and the quantification of both the chemical and electrical characteristics of molecules. They created structures using specific degree-based indices, facilitating the determination of their individual entropies. The (QSPR) of non-steroidal anti-inflammatory drugs (NSAIDs) were explored in [13]. To achieve this, the authors utilized topological indices and examined the NSAIDs data. Furthermore, they probed the QSPR analysis concerning topological indices, and the findings indicated a notable correlation between these indices and the physical attributes of chemical compounds employed in producing pain-relief medications. In [14], Hadamard symmetry and dynamic computational techniques were used, to derive a wide range of topological indices, spectral properties, and polynomials for n-dimensional hypercubes. They also analyzed the numerical properties of distance degree sequence vectors for hypercubes of up to 108 dimensions, revealing distribution patterns akin to n-cube spectra.

Poulik et al. [15] introduced the Randić index for bipolar fuzzy graphs and bipolar fuzzy subgraphs, accompanied by their inherent properties. They explored the upper and lower limits of the Randić index for bipolar fuzzy graphs, examining certain isomorphic characteristics. They investigated directed bipolar fuzzy graphs, introducing the Randić index into this framework. Furthermore, they presented various formulae for computing the Randić index for distinct categories of regular bipolar fuzzy graphs and bipolar fuzzy cycles. In [16], the authors carried out an investigation of connectivity concepts in bipolar fuzzy incidence graphs. In [17], Afzal et al. calculated the M-polynomial for a structure formed by fusing a zigzag-edged coronoid with a starphene. Additionally, they explored a range of topological indices associated with this graph, employing its M-polynomial for analysis. Akhter et al. [18] computed the harmonic polynomial and harmonic index of silicon carbide graphs. Moreover, revan indices and revan polynomials of silicon carbide graphs were investigated in [19]. The authors determined the novel degree-based topological characteristics of bismuth tri-iodide, using the M-polynomial in [20]. Kosari et al. [21] formulated an optimal lower limit for the KG-Sombor index of trees, considering both their order and maximum degree. In [22], the authors investigated some bounds of the Zagreb spectral radius (by considering factors such as the maximum degree, the minimum degree of G), the Randić index, and the first Zagreb index. These papers delved into various aspects and developments related to degree-based topological indices, providing valuable insights and updates in the field. By comprehending and utilizing topological indices effectively, researchers can unlock a deeper understanding of molecular structures, predict properties and behaviors, and accelerate the discovery and design of novel materials and compounds. Through this article, we aim to provide a valuable resource for researchers and practitioners in the field, fostering a broader utilization of topological indices and inspiring further advancements in molecular and graph analysis. Inspired by the aforementioned studies, the subsequent section focuses on exploring specific topological indices associated with a particular class of graphs, namely the flabellum graphs.

Organization

This paper is organized as follows: In Section 2, the edge partition of the flabellum graph is given and, with the help of this edge partition, general Randi¸ atom-bond connectivity, geometric–arithmetic, Zagreb, harmonic, sum connectivity, augmented Zagreb, inverse sum, and symmetric division degree indices are computed. Moreover, for these mentioned indices, corollaries are obtained, which are the indices for the Dutch windmill graph, which is a special case of the flabellum graph. In addition, the graphical representation of the indices of the Dutch windmill for the parameters n and k is given after each corollary. Section 3 features a graphical representation of the indices of the flabellum graph for the parameters n, k, and j. Then, application and comparative analysis are discussed. In the last section, there is a conclusion.

2. Main Results

The flabellum graph denoted by $F_n^{(k,j)}$ was first introduced in [23]. This graph can be obtained by considering the $k \geq 2$ duplicates of the cycle graph C_n, with each copy sharing a common central vertex, and then, in j duplicates of the cycle graph, putting an additional edge between the central vertex and each non-adjacent vertex, for $0 \le j \le k$. This construction yields the flabellum graph $F_n^{(k,j)}$, as depicted in Figure 1. The cardinality of the vertex and the edge set of the flabellum graph is $k(n-1)+1$ and $kn + nj - 3j$, respectively. Note that, for $j = 0$, the family becomes the family of Dutch windmill graphs, as shown in Figure 2. Moreover, for $n = 3$, this will become a family of friendship graphs. Table 1 gives the edge types of the flabellum graph $F_n^{(k,j)}$, and Table 2 gives the edge types of the windmill graph $D_n^{(k)}$.

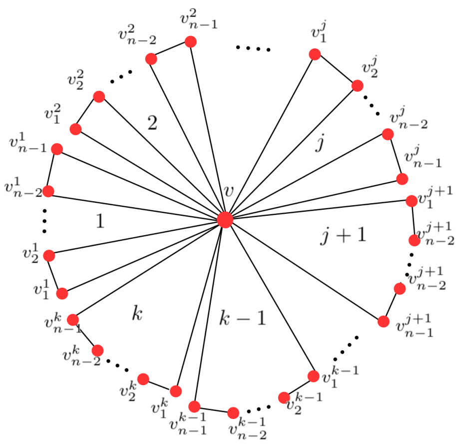


Figure 1. Flabellum graph $F_n^{(k,j)}$.

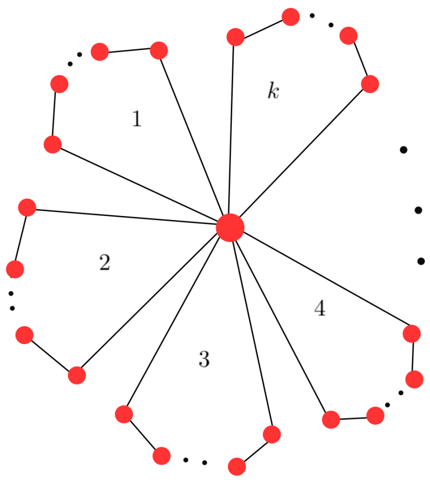


Figure 2. Dutch windmill graph $D_n^{(k)}$, with k number of copies of cycle graph having length n.

Table 1. Partition of the edges of $F_n^{(k,j)}$.

Set of Edges	Frequency
$E_{2,2}$	$(kn - jn - 2k + 2j)$
$E_{2,3}$	$2j$
$E_{3,3}$	$j(n-4)$
$E_{2k+(nj-3j),2}$	$2k$
$E_{2k+(nj-3j),3}$	$(nj - 3j)$

Table 2. Partition of the edges of $F_n^{(k,0)} = D_n^{(k)}$.

Set of Edges	Frequency
$E_{2,2}$	$k(n-2)$
$E_{2k,2}$	$2k$

2.1. Randić Index of Flabellum Graph

Milan Randic proposed the first degree-based topological index in his seminar presentation "on characterization of molecular branching [6]" in 1975. Consider the simple graph $\mathtt{G} = (\mathtt{V}, \mathtt{E})$, where, if d_u is the degree of the vertex u, then the Randić index is defined as

$$R_{-\frac{1}{2}}(\mathtt{G}) = \sum_{uv \in \mathtt{E}} \frac{1}{\sqrt{d_u d_v}}.$$

In 1988, Bollobás et al. [24], as well as Amic et al. [25], independently put forward the concept of the general Randić index, with the help of α, any non-zero real number. For further information about the Randić index (or connectivity index), including its properties and crucial findings, refer to [26,27]. The general Randić index is defined as

$$R_\alpha(\mathtt{G}) = \sum_{uv \in \mathtt{E}} (d_u d_v)^\alpha.$$

In the following theorem, the general Randić index is calculated for different values of α:

Theorem 1. *Let $F_n^{(k,j)}$ be the flabellum graph; then, the general Randić index is*

$$R_\alpha(F_n^{(k,j)}) = \begin{cases} 3j^2n^2 + \big(-18j^2 + 10jk + 5j + 4k\big)n + 27j^2 - 16j - 30jk + 8k^2 - 8k, & \text{if } \alpha = 1; \\ \frac{1}{4}(kn - jn - 2k + 2j) + \frac{3j + j(n-4)}{9} + \frac{k}{2k + nj - 3j} + \frac{(nj-3j)}{6k + 3(nj - 3j)}, & \text{if } \alpha = -1; \\ 2(kn - jn - 2k + 2j) + \big(2\sqrt{6} + 3n - 12\big)j + 2k\sqrt{4k + 2(nj - 3j)} + (nj - 3j)\sqrt{6k + 3(nj - 3j)}, & \text{if } \alpha = \frac{1}{2}; \\ \frac{1}{2}(kn - jn - 2k + 2j) + j(\frac{1}{3}\sqrt{6} + \frac{1}{3})(n-4) + \frac{k}{\sqrt{2k + nj - 3j}} + \frac{(nj-3j)}{\sqrt{6k + 3(nj - 3j)}}, & \text{if } \alpha = -\frac{1}{2}. \end{cases}$$

Proof. Consider the flabellum graph $F_n^{(k,j)}$. The edge set of $F_n^{(k,j)}$ can be partitioned into different sets, based on the degree of vertices, as shown in Table 1. Then, the general Randić index for $\alpha = 1$ is

$$\begin{aligned} R_1(F_n^{(k,j)}) &= \sum_{uv \in \mathtt{E}} (d_u d_v) \\ &= (kn - jn - 2k + 2j) \cdot (2 \cdot 2) + 2j \cdot (2 \cdot 3) + j(n-4) \cdot (3 \cdot 3) \\ &\quad + 2k \cdot (2(2k + (nj - 3j))) + (nj - 3j) \cdot (3(2k + (nj - 3j))) \\ &= 3j^2n^2 + \Big(-18j^2 + 10jk + 5j + 4k\Big)n + 27j^2 - 30jk + 8k^2 - 16j - 8k. \end{aligned}$$

For $\alpha = -1$,

$$\begin{aligned} R_{-1}(F_n^{(k,j)}) &= \sum_{uv \in \mathtt{E}} (d_u d_v)^{-1} \\ &= (kn - jn - 2k + 2j) \cdot \frac{1}{2 \cdot 2} + 2j \cdot \frac{1}{2 \cdot 3} + j(n-4) \cdot \frac{1}{3 \cdot 3} \\ &\quad + 2k \cdot \frac{1}{2(2k + (nj - 3j))} + (nj - 3j) \cdot \frac{1}{3(2k + (nj - 3j))} \\ &= \frac{1}{4}(kn - jn - 2k + 2j) + \frac{3j + j(n-4)}{9} + \frac{k}{2k + nj - 3j} + \frac{(nj - 3j)}{6k + 3(nj - 3j)}. \end{aligned}$$

For $\alpha = \frac{1}{2}$,

$$
\begin{aligned}
R_{\frac{1}{2}}(F_n^{(k,j)}) &= \sum_{uv \in E} \sqrt{d_u d_v} \\
&= (kn - jn - 2k + 2j) \cdot \sqrt{2 \cdot 2} + 2j \cdot \sqrt{2 \cdot 3} + j(n-4) \cdot \sqrt{3 \cdot 3} \\
&\quad + 2k \cdot \sqrt{2(2k + (nj - 3j))} + (nj - 3j) \cdot \sqrt{3(2k + (nj - 3j))} \\
&= 2(kn - jn - 2k + 2j) + \left(2\sqrt{6} + 3n - 12\right) j + 2k\sqrt{4k + 2(nj - 3j)} \\
&\quad + (nj - 3j)\sqrt{6k + 3(nj - 3j)}.
\end{aligned}
$$

For $\alpha = -\frac{1}{2}$,

$$
\begin{aligned}
R_{-\frac{1}{2}}(F_n^{(k,j)}) &= \sum_{uv \in E} \frac{1}{\sqrt{d_u d_v}} \\
&= (kn - jn - 2k + 2j) \cdot \frac{1}{\sqrt{2 \cdot 2}} + 2j \cdot \frac{1}{\sqrt{2 \cdot 3}} + j(n-4) \cdot \frac{1}{\sqrt{3 \cdot 3}} \\
&\quad + 2k \cdot \frac{1}{\sqrt{2(2k + (nj - 3j))}} + (nj - 3j) \cdot \frac{1}{\sqrt{3(2k + (nj - 3j))}} \\
&= \frac{1}{2}(kn - jn - 2k + 2j) + \frac{1}{3} j\sqrt{6} + \frac{1}{3}(n-4)j + \frac{k}{\sqrt{2k + nj - 3j}} \\
&\quad + \frac{(nj - 3j)}{\sqrt{6k + 3(nj - 3j)}}.
\end{aligned}
$$

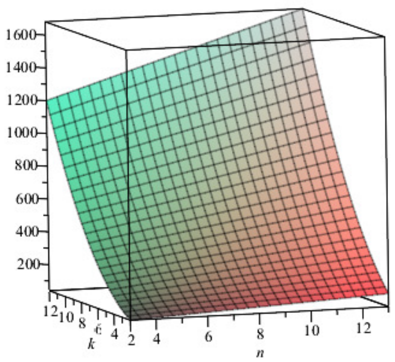
□

If we put $j = 0$ in the formula of $R_\alpha(F_n^{(k,j)})$ for α is equal to $1, -1, \frac{1}{2}$, and $-\frac{1}{2}$, the following corollary gives the formula for $R_\alpha(D_n^{(k)})$:

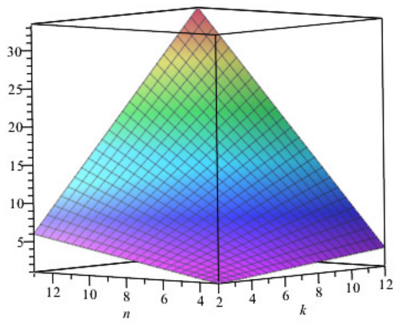
Corollary 1. *For the Dutch windmill graph $D_n^{(k)}$,*

$$
R_\alpha(D_n^{(k)}) = \begin{cases} 8k^2 + (4n - 8)k, & \text{if } \alpha = 1; \\ \frac{1}{4}k(n-2) + \frac{1}{2}, & \text{if } \alpha = -1; \\ 2k(n-2) + 2k^{3/2}\sqrt{4}, & \text{if } \alpha = \frac{1}{2}; \\ \frac{(n-2)k + 2\sqrt{k}}{2}, & \text{if } \alpha = -\frac{1}{2}. \end{cases}
$$

Note that the Randić index of the $R_{-\frac{1}{2}}(F_n^{(k,0)}) = \frac{(n-2)k+2\sqrt{k}}{2}$, which is the Randić index of the Dutch windmill graph. A graphical presentation of the Dutch windmill graph for different values α is shown in Figures 3 and 4:

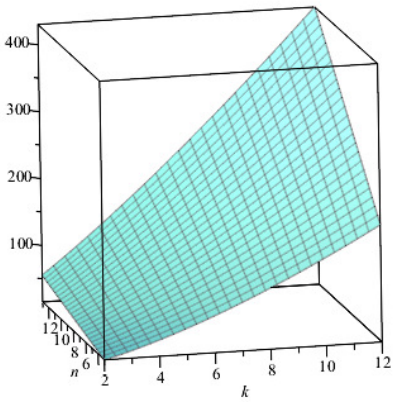


(**a**)

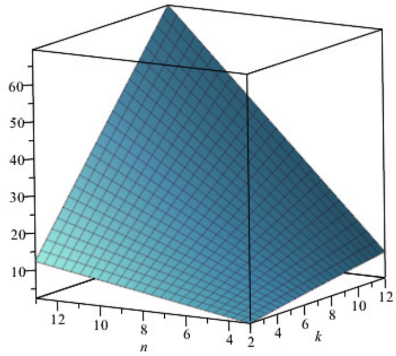


(**b**)

Figure 3. (**a**) $R_1(F_n^{(k,0)})$; (**b**): $R_{-1}(F_n^{(k,0)})$.



(**a**)



(**b**)

Figure 4. (**a**) $R_{\frac{1}{2}}(F_n^{(k,0)})$; (**b**) $R_{-\frac{1}{2}}(F_n^{(k,0)})$.

2.2. Atom-Bond Connectivity Index

The atom-bond connectivity index, known as the ABC index, is a molecular descriptor based on degrees, and was introduced by Estrada et al. [28] in the late 1990s. It has been utilized to investigate the stability of alkanes and the strain energy of cycloalkanes. For a graph $\mathtt{G}$, the ABC index is defined as

$$ABC(\mathtt{G}) = \sum_{uv\in \mathtt{E}} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}.$$

Theorem 2. *Let $\mathtt{G} \cong F_n^{(k,j)}$ be the flabellum graph; then, the ABC index is*

$$ABC(\mathtt{G}) = (j+k)\sqrt{2} + \frac{1}{\sqrt{2}}(kn - jn - 2k + 2j) + \frac{2nj - 8nj}{3} + \frac{(nj-3j)}{\sqrt{3}}\sqrt{1 + \frac{1}{2k + (n-3)j}}.$$

Proof. Consider the flabellum graph $F_n^{(k,j)}$. The edge set of $F_n^{(k,j)}$ can be partitioned into different sets, based on the degree of vertices, as shown in Table 1. For the given graph, using Table 1, we can write

$$\begin{aligned}
ABC(\mathtt{G}) &= \sum_{uv\in \mathtt{E}} \sqrt{\frac{d_u + d_v - 2}{d_u \cdot d_v}} \\
&= (kn - jn - 2k + 2j)\cdot\sqrt{\frac{2+2-2}{2\cdot 2}} + 2j\cdot\sqrt{\frac{2+3-2}{2\cdot 3}} + j(n-4)\cdot\sqrt{\frac{3+3-2}{3\cdot 3}} \\
&\quad +2k\cdot\sqrt{\frac{(2k+(nj-3j)+2-2}{2(2k+(nj-3j))}} + (nj-3j)\cdot\sqrt{\frac{(2k+(nj-3j))+3-2}{3(2k+(nj-3j))}} \\
&= (j+k)\sqrt{2} + \frac{1}{\sqrt{2}}(kn - jn - 2k + 2j) + \frac{2nj - 8nj}{3} \\
&\quad + \frac{(nj-3j)}{\sqrt{3}}\sqrt{1 + \frac{1}{2k + (n-3)j}}.
\end{aligned}$$

□

The following corollary gives the ABC index of the Dutch windmill graph. Its graphical behavior is shown in Figure 5a, with parameters k and n.

Corollary 2. *The ABC index of $F_n^{(k,0)}$ is given as*

$$ABC(F_n^{(k,0)}) = \frac{kn}{\sqrt{2}}.$$

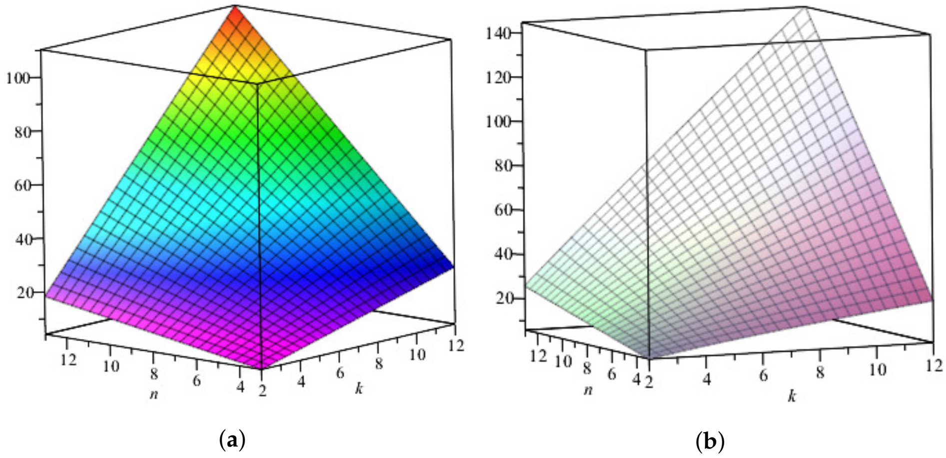


Figure 5. (**a**) $ABC(F_n^{(k,0)})$; (**b**) $GA(F_n^{(k,0)})$.

2.3. Geometric Arithmetic Index

Another significant topological index based on vertex degrees utilizes the difference between the arithmetic and the geometric means. This index, known as the geometric–arithmetic (GA) index [29], is defined as follows:

$$GA(\mathtt{G}) = \sum_{uv\in\mathtt{E}} \frac{2\sqrt{d_u d_v}}{d_u + d_v}.$$

The following theorem gives the formula of the geometric–arithmetic index:

Theorem 3. *Let $F_n^{(k,j)}$ be the flabellum graph; then,* $GA(F_n^{(k,j)}) = (kn - jn - 2k + 2j) + j(\frac{4}{5}\sqrt{6} + (n-4)) + \frac{4k\sqrt{4k+2(nj-3j)}}{2k+(nj-3j)+2} + \frac{2(nj-3j)\sqrt{6k+3(nj-3j)}}{2k+(nj-3j)+3}$.

Proof. For flabellum graph $F_n^{(k,j)}$, using the information provided in Table 1, we can compute the geometric–arithmetic index as follows:

$$\begin{aligned} GA(F_n^{(k,j)}) &= \sum_{uv\in\mathtt{E}} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \\ &= (kn - jn - 2k + 2j)\cdot\frac{2\sqrt{2\cdot 2}}{2+2} + 2j\cdot\frac{2\sqrt{2\cdot 3}}{2+3} + j(n-4)\cdot\frac{2\sqrt{3\cdot 3}}{3+3} \\ &\quad + 2k\cdot\frac{2\sqrt{(2k+(nj-3j))\cdot 2}}{2k+(nj-3j)+2} + (nj-3j)\cdot\frac{2\sqrt{2k+(nj-3j)\cdot 3}}{2k+(nj-3j)+3} \\ &= (kn - jn - 2k + 2j) + j(\frac{4}{5}\sqrt{6} + (n-4)) + \frac{4k\sqrt{4k+2(nj-3j)}}{2k+(nj-3j)+2} \\ &\quad + \frac{2(nj-3j)\sqrt{6k+3(nj-3j)}}{2k+(nj-3j)+3}. \end{aligned}$$

□

Corollary 3. *Consider $F_n^{(k,0)}$, which is a Dutch windmill graph; then,*

$$GA(F_n^{(k,0)}) = \frac{k\left(nk - 2\,k + 4\,\sqrt{k} + n - 2\right)}{k+1}.$$

Figure 5b shows the graphical depiction of the GA index of the Dutch windmill graph.

2.4. Zagreb Indices

In [7], Gutman et al. presented the concepts of Zagreb indices for the first time. They studied the link between total π-electron energy and molecule structure. These topological indices are crucial molecular descriptors and have strong relationships to a variety of chemical characteristics. The initial pair of Zagreb indices (the first and second Zagreb indices) can be described as follows:

$$\begin{aligned} M_1(\mathtt{G}) &= \sum_{v \in \mathtt{V}} d_v^2 = \sum_{uv \in \mathtt{E}} [d_u + d_v], \\ M_2(\mathtt{G}) &= \sum_{uv \in \mathtt{E}} d_u d_v. \end{aligned}$$

Theorem 4. *Let $F_n^{(k,j)}$ be the flabellum graph; then,*

- $M_1(F_n^{(k,j)}) = j^2 n^2 + \left(-6\,j^2 + (4\,k+5)j + 4\,k\right)n + 9\,j^2 + (-12\,k - 15)j + 4\,k^2 - 4\,k.$
- $M_2(F_n^{(k,j)}) = 3\,j^2 n^2 + \left(-18\,j^2 + 10\,jk + 5\,j + 4\,k\right)n + 27\,j^2 - 30\,jk + 8\,k^2 - 16\,j - 8\,k.$

Proof. From Table 1, the Zagreb indices of the flabellum graph can be computed as

$$\begin{aligned} M_1(F_n^{(k,j)}) &= \sum_{uv \in \mathtt{E}} [d_u + d_v] \\ &= (kn - jn - 2k + 2j) \cdot [2+2] + 2j \cdot [2+3] + j(n-4) \cdot [3+3] \\ &\quad + 2k \cdot [2k + (nj - 3j) + 2] + (nj - 3j) \cdot [2k + (nj - 3j) + 3] \\ &= j^2 n^2 + \left(-6\,j^2 + (4\,k+5)j + 4\,k\right)n + 9\,j^2 + (-12\,k - 15)j + 4\,k^2 - 4\,k. \end{aligned}$$

$$\begin{aligned} M_2(F_n^{(k,j)}) &= \sum_{uv \in \mathtt{E}} [d_u \cdot d_v] \\ &= (kn - jn - 2k + 2j) \cdot [2 \cdot 2] + 2j \cdot [2 \cdot 3] + j(n-4) \cdot [3 \cdot 3] \\ &\quad + 2k \cdot [2k + (nj - 3j) \cdot 2] + (nj - 3j) \cdot [2k + (nj - 3j) \cdot 3] \\ &= 3\,j^2 n^2 + \left(-18\,j^2 + 10\,jk + 5\,j + 4\,k\right)n + 27\,j^2 - 30\,jk + 8\,k^2 - 16\,j - 8\,k. \end{aligned}$$

□

The following corollary gives the formulae of the first and second Zagreb indices of the Dutch windmill graph. The graphical behavior of these indices is shown in Figure 6, where the upper and lower sheets depict the behavior of the second and the first Zagreb indices, respectively.

Corollary 4. *Let $\mathtt{G} \cong F_n^{(k,0)}$; then,*

- $M_1(\mathtt{G}) = 4k(n-2) + 2k(2k+2),$
- $M_2(\mathtt{G}) = 4k(n-2) + 8k^2.$

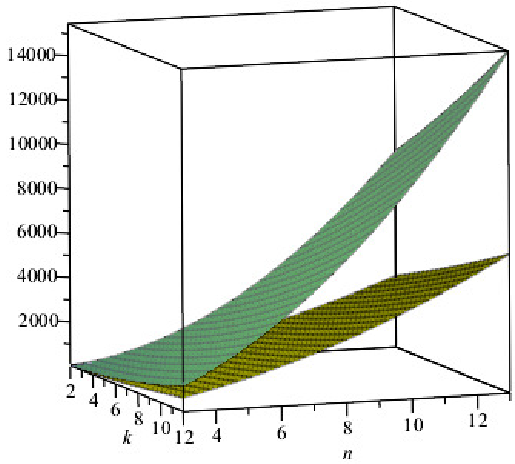


Figure 6. Graphical presentation of the first and second Zagreb indices.

2.5. Harmonic Index

The harmonic index is one of the significant degree-based topological indices, which are widely used in the domain of mathematical chemistry. In 1980, Fajtlowicz [30] introduced this index. The harmonic index of a simple graph $\mathtt{G}$ is denoted by $H(\mathtt{G})$, and is defined as follows:

$$H(\mathtt{G}) = \sum_{uv \in \mathtt{E}(\mathtt{G})} \frac{2}{d_u + d_v}.$$

It is a modified version of the well-known Randić index. When compared to the Randić index, the harmonic index exhibits relatively stronger correlations to the chemical and physical properties of graphs. Hosmani et al. [31] investigated its chemical uses and discovered it to be a useful tool for forecasting the heat of vaporization and the critical temperatures of alkanes. The following theorem and the corollary give the harmonic index of the flabellum and of the Dutch windmill graphs, respectively.

Theorem 5. *Let $F_n^{(k,j)}$ be the flabellum graph; then,*
$H(F_n^{(k,j)}) = \frac{1}{2}(kn - jn - 2k + 2j) + j(\frac{4}{5} + \frac{1}{3}(n-4)) + \frac{4k}{2k + (nj-3j)+2} + \frac{2(nj-3j)}{2k+(nj-3j)+3}$.

Proof. For flabellum graph $F_n^{(k,j)}$, using the information provided in Table 1, the harmonic index is as follows:

$$\begin{aligned} H(F_n^{(k,j)}) &= \sum_{uv \in \mathtt{E}} \frac{2}{d_u + d_v} \\ &= (kn - jn - 2k + 2j) \cdot \frac{2}{2+2} + 2j \cdot \frac{2}{2+3} + j(n-4) \cdot \frac{2}{3+3} \\ &\quad + 2k \cdot \frac{2}{2k + (nj-3j)+2} + (nj-3j) \cdot \frac{2}{2k+(nj-3j)+3} \\ &= \frac{1}{2}(kn - jn - 2k + 2j) + j(\frac{4}{5} + \frac{1}{3}(n-4)) + \frac{4k}{2k + (nj-3j)+2} \\ &\quad + \frac{2(nj-3j)}{2k+(nj-3j)+3}. \end{aligned}$$

□

Corollary 5. *Consider the flabellum graph with $j = 0$; then,*

$$H(F_n^{(k,0)}) = \frac{k(nk - 2k + n + 2)}{2k+2}.$$

A graphical presentation of the harmonic index of the Dutch windmill graph is shown in Figure 7a.

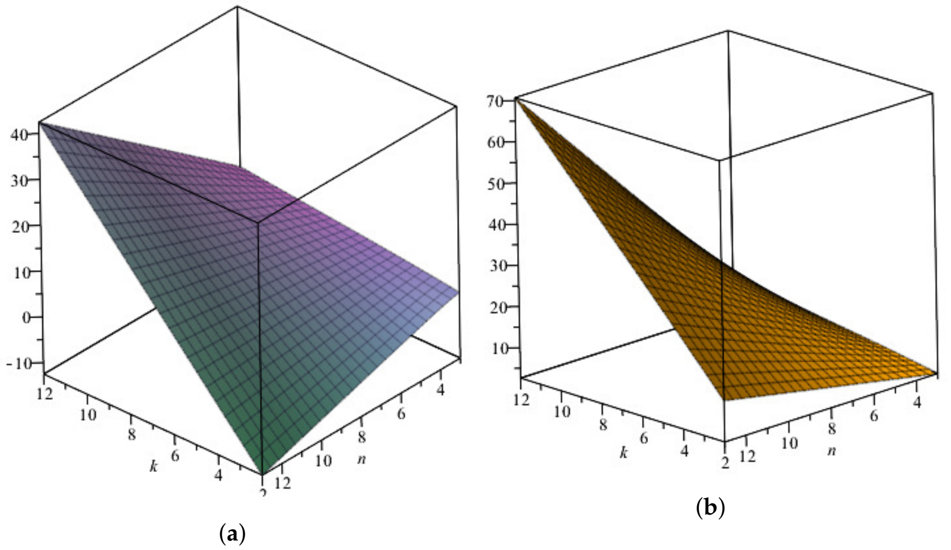


Figure 7. (**a**) $H(F_n^{(k,0)})$; (**b**) $SC(F_n^{(k,0)})$.

2.6. Sum Connectivity Index

The "sum connectivity index", a relatively new concept introduced by Bo Zhou and Nenad Trinajstic [10], is defined as follows:

$$SCI(\mathtt{G}) = \sum_{uv \in \mathtt{E}} \sqrt{\frac{1}{d_u + d_v}}.$$

Theorem 6. *Let $F_n^{(k,j)}$ be the flabellum graph; then,* $SCI(F_n^{(k,j)}) = \frac{1}{2}(kn - jn - 2k + 2j) + j(\frac{2}{\sqrt{5}} + \frac{1}{\sqrt{6}}(n-4)) + \frac{2k}{\sqrt{2k + (nj-3j) + 2}} + \frac{(nj-3j)}{\sqrt{2k+(nj-3j)+3}}$.

Proof. The sum-connectivity index for flabellum graph $F_n^{(k,j)}$, using the information provided in Table 1, can be computed as follows:

$$\begin{aligned}
SCI(F_n^{(k,j)}) &= \sum_{uv \in \mathtt{E}} \sqrt{\frac{1}{d_u + d_v}} \\
&= (kn - jn - 2k + 2j) \cdot \sqrt{\frac{1}{2+2}} + 2j \cdot \sqrt{\frac{1}{2+3}} + j(n-4) \cdot \sqrt{\frac{1}{3+3}} \\
&\quad + 2k \cdot \sqrt{\frac{1}{2k + (nj-3j) + 2}} + (nj - 3j) \cdot \sqrt{\frac{1}{2k + (nj-3j) + 3}} \\
&= \frac{1}{2}(kn - jn - 2k + 2j) + j(\frac{2}{\sqrt{5}} + \frac{1}{\sqrt{6}}(n-4)) + \frac{2k}{\sqrt{2k + (nj-3j) + 2}} \\
&\quad + \frac{(nj-3j)}{\sqrt{2k + (nj-3j) + 3}}.
\end{aligned}$$

□

Corollary 6. *Consider $F_n^{(k,0)}$; then, $SCI(F_n^{(k,0)}) = \frac{(n-2)k}{2} + \frac{k\sqrt{2}}{\sqrt{k+1}}$.*

The sum-connectivity index of the Dutch windmill graph is presented graphically in Figure 7b.

2.7. Augmented Zagreb Index

Inspired by the effectiveness of the ABC index, a modified version was introduced by Furtula et al. [32], named the "augmented Zagreb index", which is given as follows:

$$AZI(\mathtt{G}) = \sum_{uv\in\mathtt{E}} \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3.$$

Theorem 7. *Let $F_n^{(k,j)}$ be the flabellum graph; then,*

$$AZI(F_n^{(k,j)}) = 16(j+k) + 8\,(kn - jn - 2k + 2j) + \frac{(729\,n - 2916)j}{64} + \frac{27(nj-3j)(2\,k+(nj-3j))^3}{(2\,k+nj-3j+1)^3}.$$

Proof. Using the information provided in Table 1, the AZ index can be computed as

$$\begin{aligned}
AZI(F_n^{(k,j)}) &= \sum_{uv\in\mathtt{E}} \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3 \\
&= (kn - jn - 2k + 2j) \cdot \left(\frac{2\cdot 2}{2+2-2}\right)^3 + 2j \cdot \left(\frac{2\cdot 3}{2+3-2}\right)^3 \\
&\quad + j(n-4) \cdot \left(\frac{3\cdot 3}{3+3-2}\right)^3 + 2k \cdot \left(\frac{(2k+(nj-3j))\cdot 2}{2k+(nj-3j)+2-2}\right)^3 \\
&\quad + (nj-3j) \cdot \left(\frac{(2k+(nj-3j))\cdot 3}{2k+(nj-3j)+3-2}\right)^3 \\
&= 16(j+k) + 8\,(kn - jn - 2k + 2j) + \frac{(729\,n - 2916)j}{64} \\
&\quad + \frac{27(nj-3j)(2\,k+(nj-3j))^3}{(2k+nj-3j+1)^3}.
\end{aligned}$$

□

Corollary 7. *For $j = 0$,*

$$AZI(F_n^{(k,0)}) = 8k(n-2) + 16k.$$

The augmented Zagreb index can be presented graphically, as shown in Figure 8.

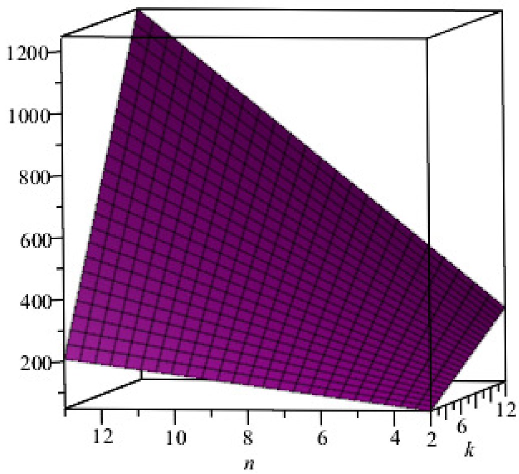


Figure 8. $AZ(F_n^{(k,0)})$.

2.8. Inverse Sum Indeg Index

Several significant degree-based topological indices are bond additive, which means they are computed by summing the contributions of individual bonds in the graph. Examples of such indices include Randić-type [26] indices and Balaban-type indices. Vukićević and Gašperov [33] examined the techniques for calculating bond partition contributions related to bond additive descriptors. They identified general concepts and utilized these concepts, to introduce a large class of molecular descriptors. These descriptors are collectively referred to as Adriatic indices. Among these descriptors, there exists a particularly intriguing subclass comprising 148 discrete Adriatic indices. These Adriatic indices have been subjected to analysis, using testing sets provided by the IMAC (International Academy of Mathematical Chemistry), and have demonstrated favorable predictive capabilities in various scenarios. Furthermore, their computer-friendly encoding makes it convenient to incorporate them into existing software packages for chemical modeling, thereby garnering significant interest in their integration. These Adriatic indices have potential implications for enhancing the efficiency and precision of numerous studies involving (QSAR) and (QSPR) [1,3].

The inverse sum indeg (ISI) index, a discrete Adriatic index, proves to be the most effective predictor of total surface area for octane isomers. The ISI index was introduced by Vukićević and Gašperov [33], and it can be written as

$$ISI(\mathtt{G}) = \sum_{uv \in \mathtt{E}(\mathtt{G})} \frac{d_u d_v}{d_u + d_v}.$$

Theorem 8. *Let $F_n^{(k,j)}$ be the flabellum graph; then,*
$ISI(F_n^{(k,j)}) = (kn - jn - 2k + 2j) + j(\frac{12}{5} + \frac{3}{2}(n-4)) + \frac{4k(2k+nj-3j)}{2k+nj-3j+2} + \frac{3j(n-3)(2k+nj-3j)}{2k+nj-3j+3}$.

Proof. For flabellum graph $F_n^{(k,j)}$, using the information provided in Table 1, we can compute the ISI index as follows:

$$\begin{aligned}
ISI(F_n^{(k,j)}) &= \sum_{uv \in \mathtt{E}} \frac{d_u d_v}{d_u + d_v} \\
&= (kn - jn - 2k + 2j) \cdot \left(\frac{2 \cdot 2}{2+2}\right) + 2j \cdot \left(\frac{2 \cdot 3}{2+3}\right) + j(n-4) \cdot \left(\frac{3 \cdot 3}{3+3}\right) \\
&\quad + 2k \cdot \left(\frac{(2k + (nj-3j)) \cdot 2}{2k + (nj-3j) + 2}\right) + (nj-3j) \cdot \left(\frac{2k + (nj-3j) \cdot 3}{2k + (nj-3j) + 3}\right) \\
&= (kn - jn - 2k + 2j) + j(\frac{12}{5} + \frac{3}{2}(n-4)) + \frac{4k(2k+nj-3j)}{2k+nj-3j+2} \\
&\quad + \frac{3j(n-3)(2k+nj-3j)}{2k+nj-3j+3}.
\end{aligned}$$

□

Corollary 8. *Consider $F_n^{(k,0)}$, which is a Dutch windmill graph; then,*

$$ISI(D_n^{(k)}) = \frac{k(nk + 2k + n - 2)}{k+1}.$$

2.9. Symmetric Division Degree Index

The symmetric division degree index (SDD) is among the 148 discrete Adriatic indices investigated by Vukičević and Gašperov in their study [33], using the benchmark data sets of IAMC. For predicting the total surface area of polychlorobiphenyls, the SDD index proves to be a highly relevant descriptor. The formula of the SDD index is as follows:

$$SDD(\mathtt{G}) = \sum_{uv \in \mathtt{E}(\mathtt{G})} \frac{d_u^2 + d_v^2}{d_u d_v}.$$

Theorem 9. *Let $F_n^{(k,j)}$ be the flabellum graph; then,*

$$SDD(F_n^{(k,j)}) = 2\,(kn - jn - 2k + 2j) + (\tfrac{13+6(n-4)}{3})j + 2\,k\Big(\tfrac{2k+(nj-3j)}{2} + \tfrac{2}{2k+nj-3j}\Big)$$
$$+(nj-3j)\Big(\tfrac{2k+nj-3j}{3} + \tfrac{3}{2k+nj-3j}\Big).$$

Proof. For flabellum graph $F_n^{(k,j)}$, using the information provided in Table 1, the SDD index can be computed as

$$\begin{aligned}
SDD(F_n^{(k,j)}) &= \sum_{uv\in \mathrm{E}} \frac{d_u^2 + d_v^2}{d_u d_v} \\
&= (kn - jn - 2k + 2j)\cdot\Big(\frac{2^2+2^2}{2\cdot 2}\Big) + 2j\cdot\Big(\frac{2^2+3^2}{2\cdot 3}\Big) + j(n-4)\cdot\Big(\frac{3^2+3^2}{3\cdot 3}\Big) \\
&\quad +2k\cdot\Big(\frac{(2k+(nj-3j))^2+2^2}{(2k+(nj-3j))\cdot 2}\Big) + (nj-3j)\cdot\frac{(2k+(nj-3j))^2+3^2}{(2k+(nj-3j))\cdot 3} \\
&= 2\,(kn - jn - 2k + 2j) + (\frac{13+6(n-4)}{3})j \\
&\quad +2\,k\Big(\frac{2k+(nj-3j)}{2} + \frac{2}{2k+(nj-3j)}\Big) \\
&\quad +(nj-3j)\Big(\frac{2k+nj-3j}{3} + \frac{3}{2k+nj-3j}\Big).
\end{aligned}$$

□

Corollary 9. *For $j = 0$, $F_n^{(k,0)} = D_n^{(k)}$; then,*

$$SDD(F_n^{(k,0)}) = 2k^2 + 2kn - 4k + 2.$$

A graphical presentation of the ISI index and the SDD index of the Dutch windmill graph is shown in Figure 9, where the lower sheet is of the ISI index and the upper sheet is of the SDD index (Table 3).

Table 3. In this table, some topological indices are computed for the flabellum graph, by giving different values to the parameters k, j, and n.

Indices	$F_4^{(5,0)}$	$F_5^{(5,1)}$	$F_6^{(5,2)}$	$F_7^{(6,3)}$
$R_{-\frac{1}{2}}$ index	7.2361	9.5244	11.600	16.096
ABC index	14.142	18.839	24.623	36.406
GA index	17.454	23.559	30.580	43.816
M_1 index	160	234	386	780
M_2 index	240	381	716	1617
H index	6.6667	8.8286	10.676	14.712
SC index	7.8867	10.492	13.156	18.519
AZ index	160	245.86	388.62	653.17
ISI index	26.667	37.843	55.736	89.854
SDD index	72	100.50	155.04	303.50

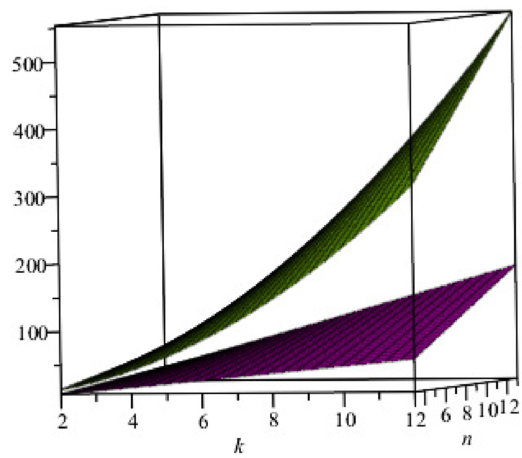
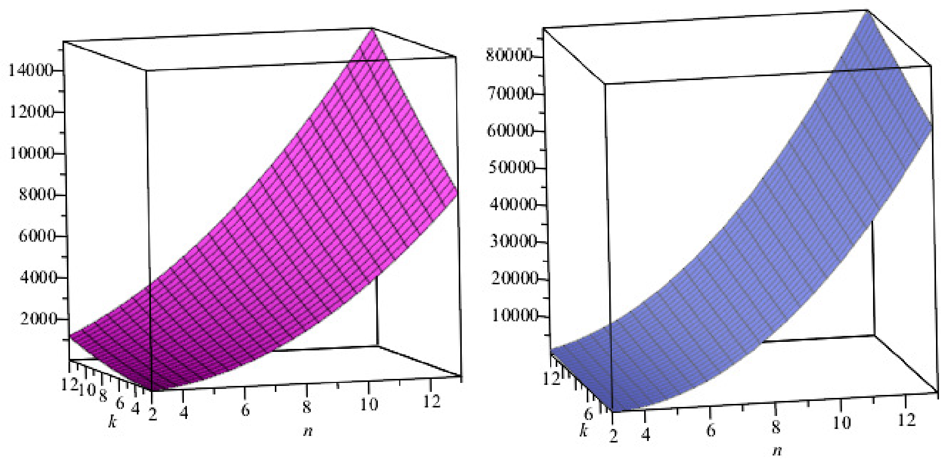


Figure 9. Graphical presentation of the ISI and SDD indices of the Dutch windmill graph.

3. Graphical Presentation of Some Degree-Based Indices of the Flabellum Graph

In this section, graphical presentations of the different degree-based topological indices of the flabellum graph are given. Figure 10 shows a graphical presentation of the general Randić index for $\alpha = 1$, $j = 5$, and $j = 15$. Figure 11 shows a graphical presentation of the general Randić index for $\alpha = -1$, $j = 5$, and $j = 15$. Figure 12 shows a graphical presentation of the general Randić index for $\alpha = \frac{1}{2}$, $j = 5$, and $j = 15$. Figure 13, shows a graphical presentation of the general Randić index for $\alpha = -\frac{1}{2}$, $j = 5$, and $j = 15$. From these graphical representations, it can be seen that for $\alpha = 1$ the general Randić index is more dominant, and that for $\alpha = -1$ the Randić index gives minimum values.

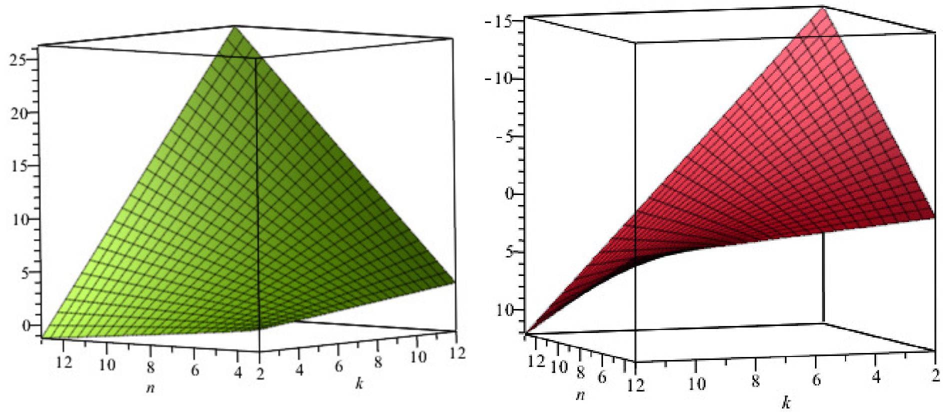
Figure 14 shows a graphical presentation of the atom-bond connectivity index for $j = 5$ and $j = 15$. Figure 15 shows a graphical presentation of the geometric–arithmetic index for $j = 5$ and $j = 15$. Figure 16 shows the graphical behavior of the first and the second Zagreb indices for the values of j: that is, 5 and 15. The upper sheet shows the behavior of the first Zagreb index, and the lower sheet shows the behavior of second Zagreb index. From these graphical representations, it can be easily seen that the second Zagreb index is more dominant than the first Zagreb index.



(**a**) (**b**)

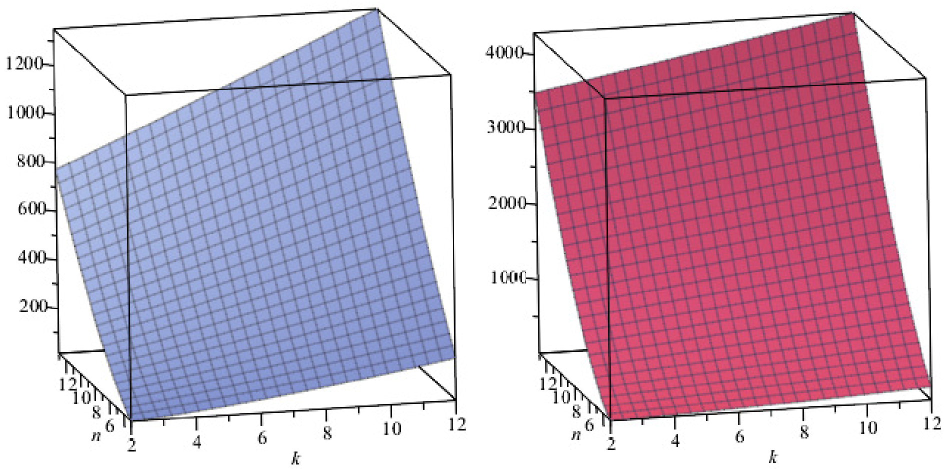
Figure 10. (**a**) $R_1(F_n^{(k,5)})$; (**b**) $R_1(F_n^{(k,15)})$.

Figures 17 and 18 show a graphical presentation of the harmonic and the sum connectivity indices for the values of $j = 5$, 15. Figure 19 shows the behavior of the augmented Zagreb index of the flabellum graph for $j = 5$ and 15. Figure 20 shows the behavior of the ISI and the SDD indices for different values of j, and it can be seen that the SDD index is more dominant. Moreover, in comparison to all the degree-based topological indices calculated in this article for the flabellum graph, the augmented Zagreb index is more dominant.



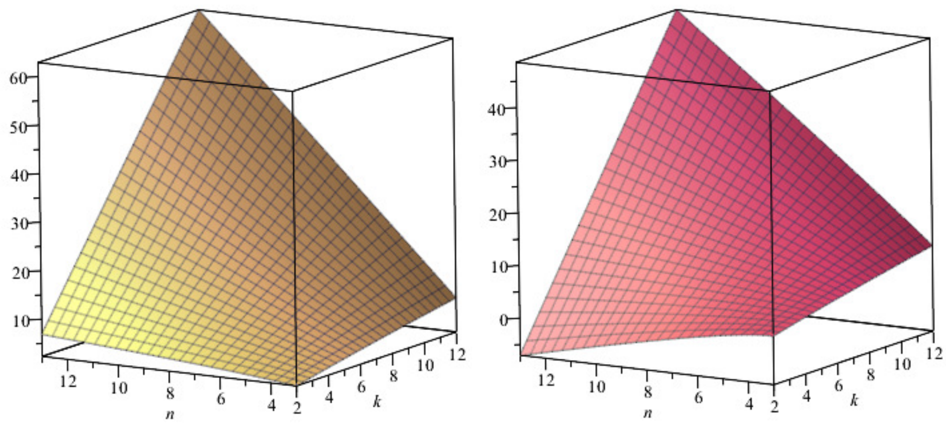
(**a**) (**b**)

Figure 11. (**a**) $R_{-1}(F_n^{(k,5)})$; (**b**) $R_{-1}(F_n^{(k,15)})$.



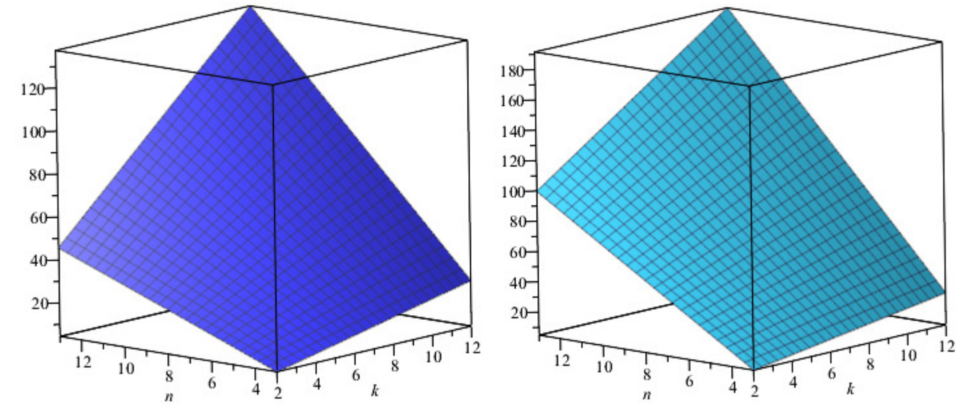
(**a**) (**b**)

Figure 12. (**a**) $R_{\frac{1}{2}}(F_n^{(k,5)})$; (**b**) $R_{\frac{1}{2}}(F_n^{(k,15)})$.



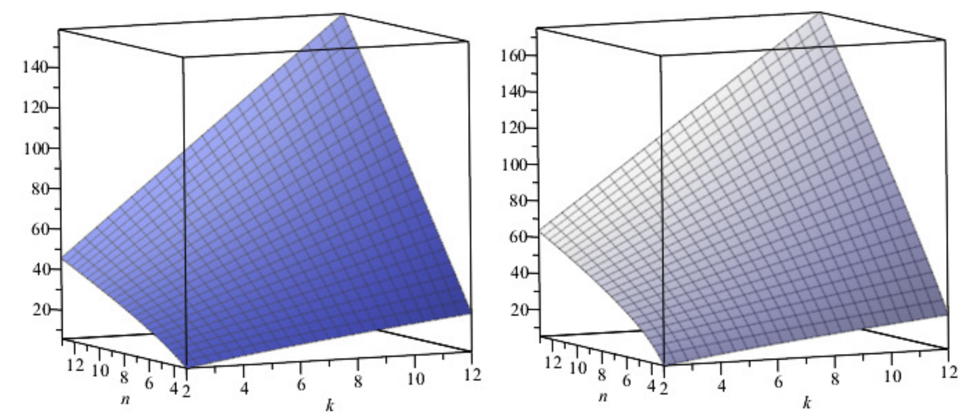
(**a**) (**b**)

Figure 13. (**a**) $R_{-\frac{1}{2}}(F_n^{(k,5)})$; (**b**) $R_{-\frac{1}{2}}(F_n^{(k,15)})$.



(**a**) (**b**)

Figure 14. (**a**) $ABC(F_n^{(k,5)})$; (**b**) $ABC(F_n^{(k,15)})$.



(**a**) (**b**)

Figure 15. (**a**) $GA(F_n^{(k,5)})$; (**b**) $GA(F_n^{(k,15)})$.

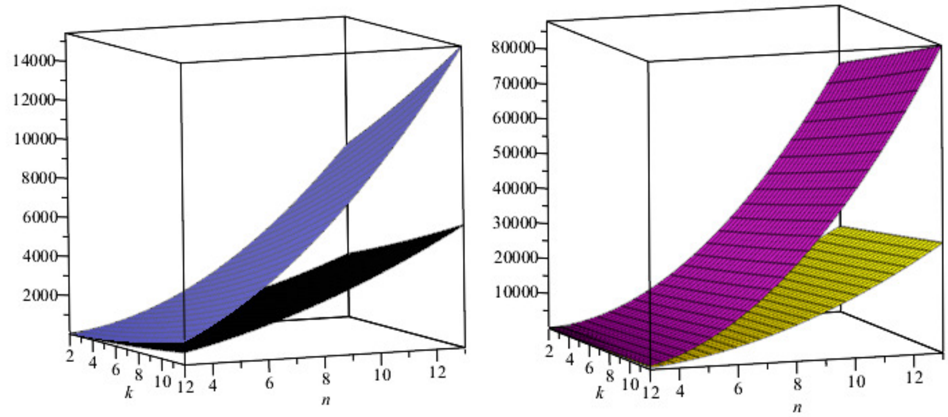
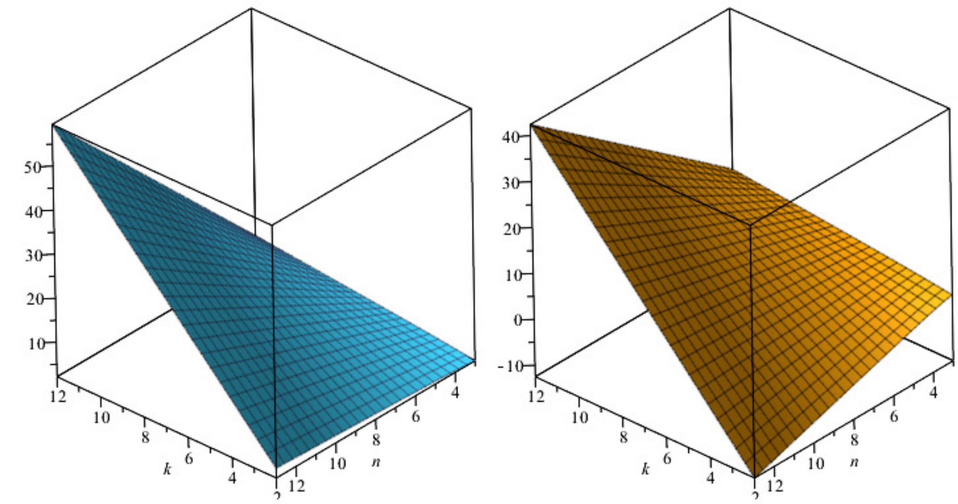
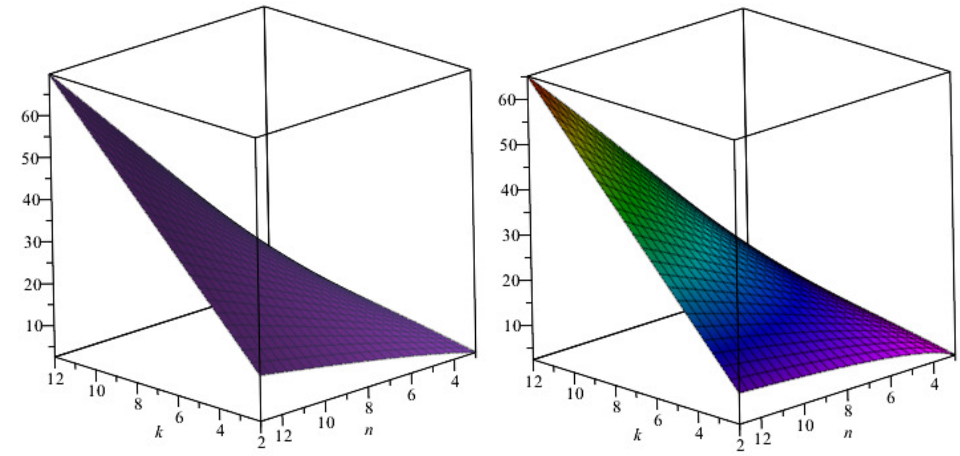


Figure 16. In the first figure, the black and blue sheets show a graphical presentation of the first Zagreb index and the second Zagreb index, respectively, of the flabellum graph for $j = 5$. In the second figure, the yellow and purple sheets show a graphical presentation of the first Zagreb index and the second Zagreb index, respectively, of the flabellum graph for $j = 15$.



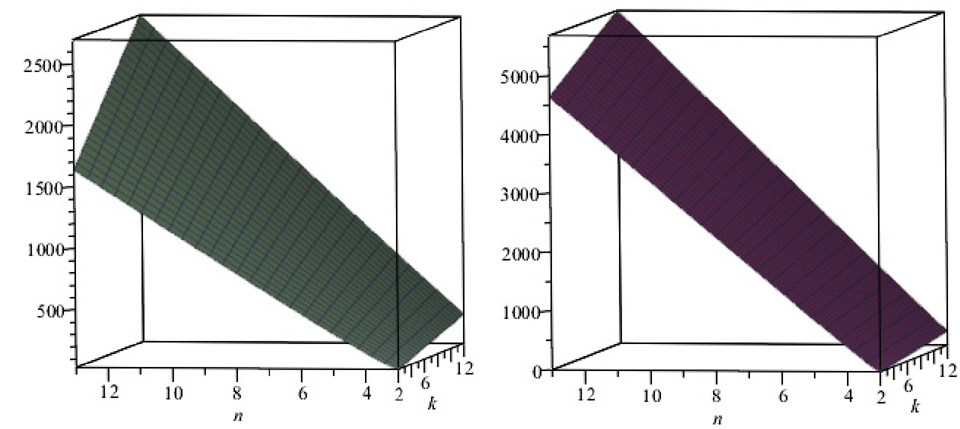
(**a**) (**b**)

Figure 17. (**a**) $H(F_n^{(k,5)})$; (**b**) $H(F_n^{(k,15)})$.



(**a**) (**b**)

Figure 18. (**a**) $SC(F_n^{(k,5)})$; (**b**) $SC(F_n^{(k,5)})$.



(**a**) (**b**)

Figure 19. (**a**) $AZ(F_n^{(k,5)})$; (**b**) $AZ(F_n^{(k,15)})$.

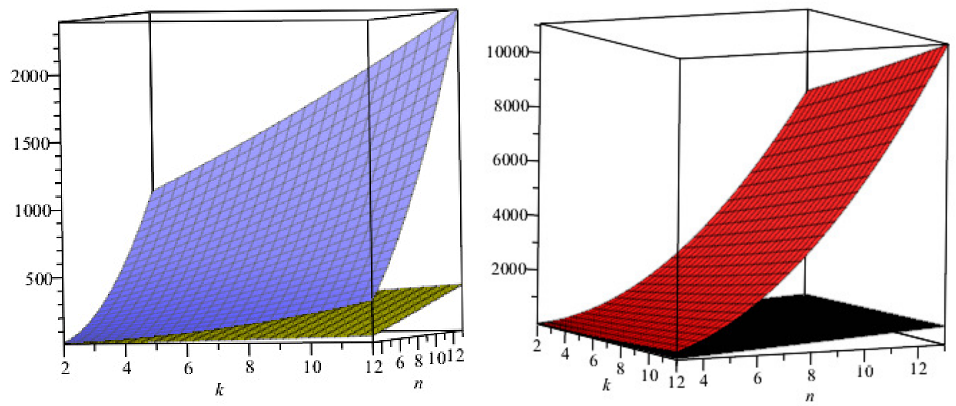


Figure 20. In the first figure, the green and blue sheets present the ISI index and the SDD index, respectively, of the flabellum graph for $j = 5$. In the second figure, the black and red sheets present the ISI index and the SDD index, respectively, of the flabellum graph for $j = 15$.

4. Application

We will use these indices to calculate the vertex closeness in a network. Vertex closeness is an important concept in network theory and has various implications in different types of networks. Closeness centrality measures how close a vertex is to all other vertices in a network, based on the length of the shortest paths. In social networks, closeness centrality is used to identify individuals who can quickly disseminate information or influence others. Those with high closeness centrality can spread information efficiently through their network. In transportation networks (like road or rail networks), closeness centrality helps identify the most central locations that provide efficient access to other parts of the network. These central locations are crucial for logistics and urban planning. Closeness centrality is vital in communication networks (like the internet). Nodes with high closeness centrality are more reliable and can serve as crucial communication hubs. Identifying such nodes helps to maintain network integrity. In biology, closeness centrality can be applied to protein–protein interaction networks. Proteins with high closeness centrality may be essential for transmitting signals efficiently within cells. In epidemiological networks, closeness centrality can help identify individuals who are likely to become infected quickly during the spread of a disease. These individuals may need special attention during disease control efforts. Cybercrime, also known as computer-based crime, encompasses unlawful activities conducted using computers and interconnected networks. Any illicit actions involving a computer, another digital device, or a computer network fall under the category of cybercrime. Pakistan ranks among the world's most active internet users. The first documented cybercrime case in Pakistan surfaced in Karachi in 2003. In 2019, the Federal Investigation Agency of Pakistan recorded 15,038 instances of cybercrime. Cybercrime can exert a substantial influence on society, manifesting in economic disruptions and psychological distress, and even posing a significant threat to national defense. Cybercriminals often operate collaboratively within groups, maintaining social connections with other wrongdoers, enabling the exchange of illicit activities. Therefore, it is crucial to pinpoint individuals within this network who exhibit more extensive interactions with fellow criminals.

Consider the flabellum graph as a cybercrime social network of 13 criminals, where the vertices $v_1, v_2, \ldots, v_{13}$ represent individuals involved in criminal activities and an edge connects two individuals if they are associated with the same type of crime. The network is shown in Figure 21. Utilizing one of the topological indices—that is, the first Zagreb index—we can identify a particularly active criminal who maintains numerous connections with other individuals involved in criminal activities. The algorithm for calculating the first Zagreb index of each vertex (criminal) is outlined in Algorithm 1. The individual corresponding to the vertex with the highest value of the first Zagreb index is deemed the most active criminal. Table 4 provides the first index values for each vertex in the flabellum criminal graph with 13 vertices.

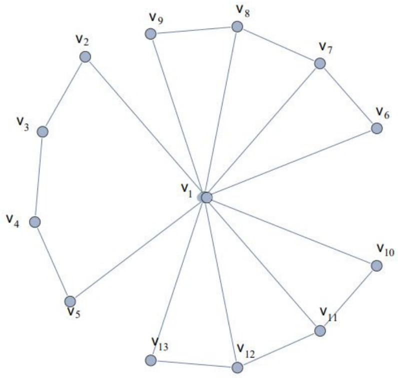


Figure 21. Data of criminals as flabellum graph $F_5^{(3,2)}$.

Algorithm 1 Algorithm to determine the first Zagreb index of the vertices of a graph.

Input: graph $G = (V, E)$.
Output: First Zagreb index of graph G
and every vertex of the graph.
1. Compute the degree of each vertex of graph G
2. Compute the first Zagreb index of the graph as
$M_1(\mathtt{G}) = \sum_{v \in \mathtt{V}} d_v^2 = \sum_{uv \in \mathtt{E}} [d_u + d_v]$.
3. Make subgraph G_v by deleting vertex v
for each $v \in V(G)$, and then calculate $M_1(G_v)$.
4. Compute the first Zagreb index of vertex v as
$M_1(v) = M_1(G) - M_1(G_v)$.
5. End.

It is evident from this table that vertex 'v_1' possesses the highest value, signifying that 'v_1' is in closer proximity to all other vertices, compared to the rest. In essence, 'v_1' emerges as the most interconnected criminal among the 13 individuals under scrutiny.

Table 4. First Zagreb index of each vertex of the criminal network graph $F_5^{(3,2)}$.

Vertices, v_i	$M_1(v_i)$
v_1	138
v_2	26
v_3	10
v_4	10
v_5	26
v_6	28
v_7	36
v_8	36
v_9	28
v_{10}	28
v_{11}	36
v_{12}	36
v_{13}	28

5. Comparative Analysis

To make a comparison, we examined the cybercrime scenario discussed in the previous section, and we compared the first Zagreb index values of the vertices to those obtained from existing models, such as the closeness centrality measure. Our analysis demonstrates the effectiveness of our proposed method. It is evident that computing degrees is a simpler task, compared to determining the distances between each vertex and all other vertices. Therefore, calculating distances can significantly complicate the process, especially in the context of large networks. In such cases, our proposed method can provide valuable assistance. Table 5 illustrates that 'v_1' exhibits the highest closeness centrality measure and the highest value of the first Zagreb index. High closeness centrality indicates that a v_1 criminal has quick access to information, resources, or other members within the network. In the context of cybercrime, these individuals might be key players who can efficiently coordinate and carry out cybercriminal activities. An illustration of the network is shown in Figure 22, where the thickness of each vertex (or criminal) shows the activeness of that vertex (or criminal).

Table 5. First Zagreb index and closeness centrality of each vertex in the criminal network shown in Figure 21.

Vertices	Fist Zagreb Index	Closeness Centrality
v_1	138	0.857143
v_2	26	0.545455
v_3	10	0.4
v_4	10	0.4
v_5	26	0.545455
v_6	28	0.5
v_7	36	0.521739
v_8	36	0.521739
v_9	28	0.5
v_{10}	28	0.5
v_{11}	36	0.521739
v_{12}	36	0.521739
v_{13}	28	0.5

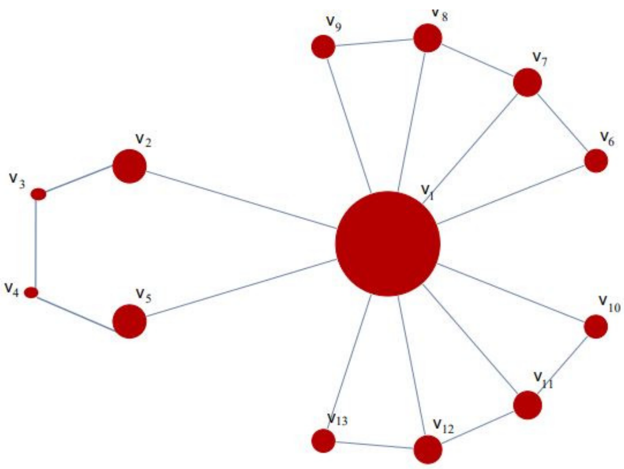


Figure 22. In this network, the thickness of each vertex shows how active is that criminal.

6. Conclusions

Graph theory has equipped chemists with a range of highly valuable tools, enabling the prediction of numerous intriguing physical and chemical characteristics of studied materials. The exploration of various topological indices across different graph structures opens up wide avenues for theoretical exploration and practical applications, with a significant impact on the understanding of chemical structures and their characteristics. This research narrowed its focus to specific vertex-degree-based topological indices, particularly within the unique realm of flabellum graphs. Additionally, this study not only computed but also visually represented these degree-based topological indices, enhancing our insights into their behavior within this specific graph class. Moreover, the fuzzy first Zagreb index was applied to the problem of cybercrime, aiming to investigate the branching patterns within a cyber flabellum graph involving 13 criminals. By utilizing the first Zagreb index for the vertices (representing criminals) within the cyber graph, we were able to identify the most active criminal. An algorithm was also introduced, for calculating the first Zagreb index values for the graph's vertices. A higher first Zagreb index value for a vertex indicated a greater level of involvement in cybercriminal activities with other criminals. Furthermore, a comparative analysis was conducted to existing closeness centrality measures, which found that our approach was in concordance with these established methods. Compared to more established graph types, the properties and applications of flabellum graphs are relatively less explored, which can limit the availability of existing research and tools. Their construction involves additional edges between a central vertex and non-adjacent vertices in duplicated cycle graphs. This complexity can make them challenging to analyze, compared to simpler graph structures. Despite these limitations, flabellum graphs serve as a valuable subject for specific theoretical investigations and contribute to the diversity of graph theory.

Author Contributions: Conceptualization, X.S., S.K., U.A., S.H. and S.A. All authors have read and agreed to the published version of the manuscript.

Funding: This work was supported by the National Key R&D Program of China (Grant 2019YFA0706402) and by the National Natural Science Foundation of China under Grants 62172302, 62072129, and 61876047.

Data Availability Statement: Data will be available on request.

Conflicts of Interest: The authors declare no conflict of interest.

References

1. Karelson, M. *Molecular Descriptors in QSAR/QSPR*; Wiley-Inter Science: New York, NY, USA, 2000.
2. Estrada, E.; Guevara, N.; Gutman, I.; Rodriguez, L. Molecular connectivity indices of iterated line graphs. A new source of descriptors for QSPR and QSAR studies. *SAR QSAR Environ. Res.* **1998**, *9*, 229–240. [CrossRef]
3. Devillers, J.; Balaban, A.T. *Topological Indices and Related Descriptors in QSAR and QSPAR*; Gordon and Breach: Amsterdam, The Netherlands, 1999.
4. Aguero-Chapin, G.; Antunes, A.; Ubeira, F.M.; Chou, K.C.; Gonzalez-Diaz, H. Comparative study of topological indices of macro/supramolecular RNA complex networks. *J. Chem. Inf. Model.* **2008**, *48*, 2265–2277. [CrossRef] [PubMed]
5. Gutman, I.; Estrada, E. Topological indices based on the line graph of the molecular graph. *J. Chem. Inf. Comput. Sci.* **1996**, *36*, 541–543. [CrossRef]
6. Randić, M. Characterization of molecular branching. *J. Am. Chem. Soc.* **1975**, *97*, 6609–6615. [CrossRef]
7. Gutman, I.; Trinajstić, N. Graph theory and molecular orbitals. Total ϕ-electron energy of alternant hydrocarbons. *Chem. Phys. Lett.* **1972**, *17*, 535–538. [CrossRef]
8. Zhou, B.; Trinajstić, N. Bounds on the Balaban index. *Croat. Chem. Acta* **2008**, *81*, 319–323.
9. Gutman, I.; Vidović, D.; Furtula, B. Coulson function and Hosoya index. *Chem. Phys. Lett.* **2002**, *355*, 378–382. [CrossRef]
10. Zhou, B.; Trinajstić, N. On a novel connectivity index. *J. Math. Chem.* **2009**, *46*, 1252–1270. [CrossRef]
11. Chaluvaraju, B.; Boregowda, H.S.; Diwakar, S.A. Hyper-Zagreb indices and their polynomials of some special kinds of windmill graphs. *Int. J. Adv. Math.* **2017**, *4*, 21–32.
12. Ghani, M.U.; Campena, F.J.H.; Ali, S.; Dehraj, S.; Cancan, M.; Alharbi, F.M.; Galal, A.M. Characterizations of Chemical Networks Entropies by K-Banhatii Topological Indices. *Symmetry* **2023**, *15*, 143. [CrossRef]
13. Gnanaraj, L.R.M.; Ganesan, D.; Siddiqui, M.K. Topological indices and QSPR analysis of NSAID drugs. *Polycycl. Aromat. Compd.* **2023**, 1–17. [CrossRef]
14. Balasubramanian, K. Topological indices, graph spectra, entropies, Laplacians, and matching polynomials of n-dimensional hypercubes. *Symmetry* **2023**, *15*, 557. [CrossRef]

15. Poulik, S.; Das, S.; Ghorai, G. Randic index of bipolar fuzzy graphs and its application in network systems. *J. Appl. Math. Comput.* **2022**, *68*, 2317–2341. [CrossRef]
16. Poulik, S.; Ghorai, G. Connectivity Concepts in Bipolar Fuzzy Incidence Graphs. *Thai J. Math.* **2022** *20*, 1609–1619.
17. Afzal, F.; Hussain, S.; Afzal, D.; Hameed, S. M-polynomial and topological indices of zigzag edge coronoid fused by starphene. *Open Chem.* **2020**, *18*, 1362–1369. [CrossRef]
18. Akhter, S.; Ashraf, R. Harmonic Polynomial and Harmonic Index of Silicon Carbide Graphs SiC_3-I and SiC_3-II. *Int. J. Fuzzy Math. Syst.* **2019**, *17*, 83–89. [CrossRef]
19. Ashraf, R.; Akhter, S. Revan indices and revan polynomials of silicon carbide graphs. *Int. J. Eng. Res. Technol.* **2019**, *8*, 353–361.
20. Hameed, S.; Husin, M.N.; Afzal, F.; Hussain, H.; Afzal, D.; Farahani, M.R.; Cancan, M. On computation of newly defined degree-based topological invariants of Bismuth Tri-iodide via M-polynomial. *J. Discrete Math. Sci. Cryptogr.* **2021**, *24*, 2073–2091. [CrossRef]
21. Kosari, S.; Dehgardi, N.; Khan, A. Lower bound on the KG-Sombor index. *Commun. Comb. Optim.* **2023**, *8*, 751–757.
22. Kosari, S. On spectral radius and Zagreb Estrada index of graphs. *Asian-Eur. J. Math.* **2023**. [CrossRef]
23. Guan, H.; Khan, A.; Akhter, S.; Hameed, S. Spectral Characterization of Graphs with Respect to the Anti-Reciprocal Eigenvalue Property. *Symmetry* **2023**, *15*, 1240. [CrossRef]
24. Bollobás, B.; Erdös, P. Graphs of extremal weights. *Ars Comb.* **1998**, *50*, 225. [CrossRef]
25. Amić, D.; Bešlo, D.; Lucić, B.; Nikolić, S.; Trinajstić, N. The vertex-connectivity index revisited. *J. Chem. Inf. Comput.* **1998**, *38*, 819–822. [CrossRef]
26. Li, X.; Gutman, I. *Mathematical Aspects of Randić type Molecular Structure Descriptors*; Mathematical Chemistry Monographs No. 1; University of Kragujevac: Kragujevac, Serbia, 2006; p. 330.
27. Shao, Z.; Siddiqui, M.K.; Muhammad, M.H. Computing Zagreb indices and Zagreb polynomials for symmetrical nanotubes. *Symmetry* **2018**, *10*, 244. [CrossRef]
28. Estrada, E.; Torres, L.; Rodriguez, L.; Gutman, I. An Atom-Bond Connectivity Index: Modelling the Enthalpy of Formation of Alkanes. *Indian J. Chem.* **1998**, *37A*, 849–855.
29. Vukičević, D.; Furtula, B. Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges. *J. Math. Chem.* **2009**, *46*, 1369–1376. [CrossRef]
30. Fatlowicz, S. On conjectures of Graffiti. *Congr. Nummerantium* **1987**, *60*, 187–197.
31. Hosamani, S.; Perigidad, D.; Jamagoud, S.; Maled, Y.; Gavade, S. QSPR analysis of certain degree based topological indices. *J. Stat. Appl.* **2017**, *6*, 361–371. [CrossRef]
32. Furtula, B.; Graovac, A.; Vukičević, D. Augmented zagreb index. *J. Math. Chem.* **2010**, *48*, 370–380. [CrossRef]
33. Vukičević, D.; Gašperov, M. Bond additive modeling 1. Adriatic indices. *Croat. Chem. Acta* **2010**, *83*, 243.