JURNAL MATEMATIKA, STATISTIKA DAN KOMPUTASI e–ISSN: 2614–8811
Published by Departement of Mathematics, Hasanuddin University, Indonesia
https://journal.unhas.ac.id/index.php/jmsk/index
Vol. 22, No. 1, September 2025, pp. 102-113
DOI: 10.20956/j.v22i1.44688

Computing The First Zagreb Index, The Wiener Index and The Gutman Index of The Power of Dihedral Group Using Python

Komputasi Indeks Zagreb Pertama, Indeks Wiener, dan Indeks Gutman pada Power dari Grup Dihedral Menggunakan Python

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Abstract
This paper presents a computational study on three classical topological indices—the First Zagreb Index, Wiener Index, and Gutman Index—within the context of power graphs of the dihedral group D_{2n}, where n is a positive integer representing half the order of the group. These indices are fundamental in mathematical chemistry and graph theory, serving as quantitative descriptors of graph structure and connectivity. The methodology involves constructing power graphs derived from D_{2n} and calculating the indices using Python programming, supported by the NetworkX, Matplotlib, and Gradio libraries. Numerical simulations were conducted for varying values of n, revealing consistent algebraic patterns and insights into the structural complexity of the corresponding graphs. Additionally, an interactive Python-based interface is developed to facilitate real-time computation and visualization, thus promoting further exploration and application in algebraic graph theory.

Keywords: Power Graph, Dihedral Group, Topological Index, Zagreb Index, Wiener Index, Gutman Index, Python.

Abstrak
Penelitian ini menyajikan kajian komputasional terhadap tiga indeks topologi klasik—First Zagreb Index, Wiener Index, dan Gutman Index—dalam konteks graf pangkat dari grup dihedral, di mana n adalah bilangan bulat positif yang menyatakan setengah dari orde grup tersebut. Ketiga indeks ini berperan penting dalam kimia matematis dan teori graf sebagai deskriptor kuantitatif terhadap struktur dan konektivitas graf. Metodologi yang digunakan mencakup konstruksi graf pangkat dari D_{2n} serta perhitungan indeks menggunakan

pemrograman Python dengan dukungan pustaka NetworkX, Matplotlib, dan Gradio. Simulasi numerik dilakukan untuk berbagai nilai n, yang mengungkap pola aljabar yang konsisten serta memberikan wawasan mengenai kompleksitas struktural dari graf yang dihasilkan. Selain itu, dikembangkan pula antarmuka interaktif berbasis Python untuk memfasilitasi perhitungan dan visualisasi secara waktu nyata, sehingga mendorong eksplorasi dan penerapan lebih lanjut dalam teori graf aljabar.

Kata kunci: Graf Pangkat, Grup Dihedral, Indeks Topologi, Indeks Zagreb, Indeks Wiener, Indeks Gutman, Python.

1. INTRODUCTION AND PRELIMINARIES

In the realm of discrete mathematics and modern algebra, graph theory has evolved into a fundamental analytical tool for modeling abstract structures, including group representations through specific graph constructions. One such construction that has attracted significant attention is the power graph, a type of graph that represents the exponentiation relationships among group elements, where two vertices are connected if one is a power of the other [4].

Definition 1.1. [4] A *group G is said to be a dihedral group of order $2n, n \geq 3,$ and $n \in \mathbb{N}$, if it is a group composed of two elements $a, b \in G$ with the property*

$$G = \langle a, b | a^n = e, b^2 = e, bab^{-1} = a^{-1} \rangle$$

The dihedral group of order $2n$ is denoted by D_{2n}

Definition 1.2. [4] *Power graph of group G denoted by $\mathcal{G}(G)$ is an undirected graph whose vertex set is G and two vertices $a, b \in G$ are adjacent if and only if $a \neq b$ and $a^m = b$ or $b^m = a$ for some positive integer m.*

The power graph of the dihedral group not only reveals the combinatorial properties of the group but also provides a visual framework for analyzing the complexity of group operations [1]. The dihedral group D_{2n}, which represents the symmetries of a regular polygon with n sides, serves as an ideal subject of study due to its characteristic combination of rotations and reflections, as well as its rich subgroup structure [5]. Previous studies have investigated the parameters of the power graph of D_{2n} for $n = p$ (where p is a prime number), including the First Zagreb Index, the Wiener Index and the Gutman Index [1].

Theorem 1.1. [4] *If $n = p^m$ where p is a prime number and m is a natural number, then the Zagreb Index of the power graph of the dihedral group D_{2n} is $n^2(n+1)$.*

Theorem 1.2. [4] *If $n = p^m$ where p is a prime number and m is a natural number, then the Wiener Index of the power graph of the dihedral group D_{2n} is $\frac{7n^2}{2} - \frac{5n}{2}$.*

Theorem 1.3. [4] *If $n = p^m$ where p is a prime number and m is a natural number, then the Gutman Index of the power graph of the dihedral group D_{2n} is $\frac{1}{4}(n^4 + n) - \frac{3}{2}(n^3 - n^2)$.*

These three theorems demonstrate a consistent algebraic pattern associated with the prime factorization of the group order [1]. Topological indices such as the First Zagreb, Wiener, and Gutman indices not only play a central role in pure mathematics but also have interdisciplinary applications, including computational chemistry, where they are used to predict the physicochemical properties of molecules through graph representations [2].

Several researchers have proposed methods to compute these indices using both algebraic and computational approaches. Asmarani et al. [4] analytically derived the exact formulas for the First Zagreb Index, Wiener Index, and Gutman Index of the power graph of the dihedral group using closed-form expressions. Their work laid the foundation for further computational exploration. Syarifudin and Wijaya [7] developed Python-based code to generate the subgroups of D_{2n}, which can also support the structural decomposition necessary for topological index analysis. Moreover, recent advances in Python programming and algorithm design, as presented by Arifin et al. [3], have enabled the development of efficient scripts to compute graph properties, which can be adapted to automate the calculation of these indices for larger group orders. These computational implementations support scalability and allow researchers to validate theoretical results across broader data ranges.

In the context of the dihedral group, these indices serve as critical structural indicators, particularly in identifying graph partitions, connectivity, and subgroup hierarchies [4]. However, most existing studies still rely on manual or semi-formal approaches, which are prone to limitations in scalability and generalization [6]. Compared to manual derivations, Python allows flexible experimentation across a wide range of values, making it ideal for exploring index behavior beyond closed-form expressions.

Recent developments in symbolic computation, driven by the Python programming language and libraries such as Gradio, offer a new paradigm for automating the computation of complex graph parameters [3]. Python-based algorithm implementations enable the numerical validation of theoretical results, exploration of cases with large group orders ($n \geq 3$) and sensitivity analysis with respect to variations in the parameters p and m [2]. For instance, a study by Nusantara and Maulana [5] demonstrated the effectiveness of Python in solving irreducible polynomial problems and calculating GCD/LCM in finite fields, which is relevant to modular operations within dihedral groups. This integration of algebraic theory and numerical methods acts as a catalyst for extending research toward more complex non-Abelian group structures. Furthermore, the study by Gazir and Rievaldo [7] successfully developed Python code to generate all proper subgroups of the Dihedral group D_{2n} and classified the subgroups into three types: reflexive subgroups, rotational subgroups, and mixed subgroups combining both elements.

Despite significant progress in the study of group-related graphs, methodological gaps remain. Previous research on coprime graphs and power graphs of D_{2n} has mostly focused on theoretical deductions without leveraging computational tools for empirical verification or expansion of test cases. Furthermore, the limited literature examining the relationship between the prime factorization of group orders and the distribution of topological indices constrains a holistic understanding of power graph dynamics [5]. Accordingly, this study aims to:

1. Design a Python-based computational algorithm to calculate the First Zagreb Index, Wiener Index, and Gutman Index for the power graph of D_{2n} where $n = p^m$;
2. Validate the previously derived theoretical formulas through numerical simulations;
3. Explore general patterns of topological indices as functions of the parameters p and m.

The main contribution of this research lies in the synthesis of mathematical rigor and computational efficiency, which not only reinforces the theoretical foundation but also provides a practical framework for the analysis of algebraic graphs at scale.

2. MAIN RESULTS

This study was conducted through a literature review on the First Zagreb Index, Wiener Index, and Gutman Index of power graphs derived from dihedral groups. Additionally, the research includes the implementation of algorithms to compute these three indices using Python, as well as the visualization of the corresponding graphs.

Algorithm 1 (Main Controller for Dihedral Graph Indices Calculation): This serves as the main controller function which governs the process of computing graph indices for the power of dihedral group D_{2n}. The input is an integer n, where $n \geq 3$. The function validates whether n satisfies the necessary condition for constructing the power graph, which must be of the form $n = p^m$, where p is a prime number and $m \geq 1$.If valid, the function constructs the corresponding graph, calculates the First Zagreb Index, Wiener Index, and Gutman Index using predefined mathematical formulas, and optionally visualizes the graph and the indices. Otherwise, it returns an appropriate error message.

Algorithm 1 (Main Controller for Dihedral Graph Indices Calculation)

1: **Input**: Integer n for the power of dihedral group D_{2n}

2: Validate if $n \geq 3$. If not, raise an error

3: Determine whether n can be expressed as $n = p^m$, where p is a prime number. This is done using a helper function find_p_and_$m(n)$ which attempts to find a pair of integers (p, m).

4: If no such pair is found (i.e., n is not a power of a prime), return an error message stating: "Cannot find p and m for the given n"

5: If valid p and m are found, construct the power graph for D_{2n} using class PowerDihedralGraph(p, m).

6: Compute the following graph indices using methods of the class:

- zagreb_index_first() to compute First Zagreb Index.
- wiener_index() to compute Wiener Index.
- gutman_index() to compute Gutman Index.

7: **Output**: Values of p, m and the three indices. Optional visualizations are available for the graph structure and indices.

Algorithm 2 (First Zagreb, Wiener, and Gutman Index Calculation): This algorithm encapsulates the closed-form formulas for computing three graph indices on the power graph of the dihedral group D_{2n}, assuming that $n = p^m$ is valid. The computation is embedded as methods in the class PowerDihedralGraph.

Algorithm 2 Index Calculation for Valid Power Dihedral Graph

1: **Input**: Integer $n = p^m$, where p is a prime and $m \geq 1$.

2: Construct the power graph for D_{2n}.

3: Compute the First Zagreb Index using: $n^2(n + 1)$

4: Compute the Wiener Index using: $\frac{7n^2}{2} - \frac{5n}{2}$

5: Compute the Gutman Index using: $\frac{1}{4}(n^4 + n) - \frac{3}{2}(n^3 - n^2)$.

6: **Output**: The values of all three indices for given n.

Algorithm 3 (Graph Construction of the Power of Dihedral Group): This algorithm outlines how the graph is constructed based on the power structure of the dihedral group D_{2n}, using the class PowerDihedralGraph.

Algorithm 3 Construct Power Graph of D_{2n}

1: **Input**: Prime p, exponent m, such that $n = p^m$.

2: Initialize an undirected graph G.

3: Add the identity element e as a node.

4: For each $i = 1$ to $n - 1$, add node a^i

5: For each $i = 0$ to $n - 1$, add node a^ib

6: For each i, j such that $1 \leq i < j < n$, if gcd $(i, j) > 1$, connect a^i and a^j

7: For each i, j such that $0 \leq i < j < n$, if gcd $(i, j) > 1$, connect a^ib and a^jb

8: Connect e to every a^i and a^ib, where $1 \leq i < n$.

9: **Output:** Fully constructed power graph G.

Algorithm 4 (Prime Power Decomposition): This algorithm determines whether an integer n can be written as p^m, where p is a prime and $m \geq 1$. This acts as the validation for graph construction.

Algorithm 4 Find Prime p and Exponent m such that $n = p^m$

1: **Input:** Integer $n \geq 3$

2: For each integer $p \in [2, n]$:

3: Check whether p is prime.

4: For each exponent $m \geq 1$, compute p^m.

5: If $p^m = n$, return (p, m).

6: If no pair (p, m) satisfies If $p^m = n$ return None.

7: **Output**: A valid pair (p, m), or an error if not found.

Algorithm 5 (Visualization): This algorithm provides optional visual representations of the power graph and the computed indices, both for a single n and across a range of n.

Algorithm 5A Visualize Power Graph for D_{2n}

1: Use spring_layout to generate node positions for visual clarity.

2: Render the graph using matplotlib and networkx.draw.

3: Display all nodes and edges with labels.

4: **Output:** Plot showing the structure of the power graph.

Algorithm 5B Visualize Index Values for Single n

1: Compute Zagreb, Wiener, and Gutman indices for the given n

2: Plot the three Index values on a simple line graph.

3: Label each Index and axis appropriately.

4: **Output:** Single-line plot of Index values for specific n.

Algorithm 5C Visualize Index Trends for $3 \leq n \leq 50$

1: For each $n \in [3,50]$, compute:

- First Zagreb Index: $n^2(n+1)$
- Wiener Index: $\frac{7n^2}{2} - \frac{5n}{2}$
- Gutman Index: $\frac{1}{4}(n^4 + n) - \frac{3}{2}(n^3 - n^2)$.

2: Plot all three Index series on the same graph.

3: Use different markers and colors for distinction.

4: Add legends, titles, and axis labels.

5: **Output**: Comparative Index plot over a range of n

The entire technical implementation of this research has been realized using the Python programming language and is publicly accessible through the following GitHub repository: https://github.com/rarakk21/indeks-grup-dihedral-. This repository contains a comprehensive collection of scripts encompassing the construction of the power graph of the dihedral group D_{2n}, systematic computations of three topological graph indices—namely the First Zagreb Index, Wiener Index, and Gutman Index—as well as graphical visualizations derived from numerical analyses conducted over various values of the parameter n. In addition, an interactive interface developed using the Gradio framework is included to facilitate dynamic and user-friendly exploration of the results.

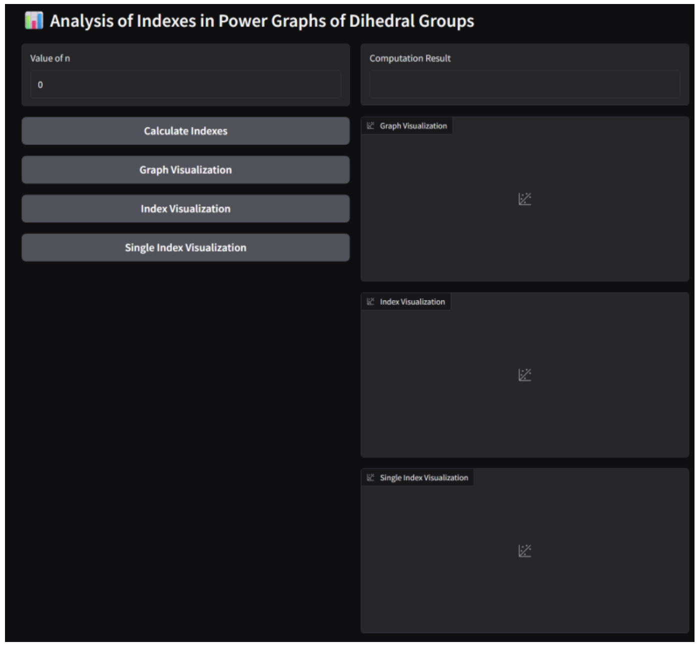

Figure 2.1. Initial Interface Display

The figure above illustrates the initial display of the Power Dihedral Graph Index Analysis application interface developed using Gradio. Below is an explanation of the elements contained within the initial interface:

1. Input Field for Value of n
   The input box located at the top-left is used to enter the value of n, which represents the order of the dihedral group D_{2n}. In the initial display, the value is set to 0, indicating that no input has been provided yet.
2. Interaction Buttons
   There are four buttons located at the bottom-left, each designed to execute a specific function within the application:
   a. Calculate Indices – Executes the computation of the First Zagreb Index, Wiener Index, and Gutman Index based on the input value of n.
   b. Graph Visualization – Displays the power graph of the dihedral group based on the given value of n.
   c. Indices Visualization – Displays a line chart comparing the three indices across a range of n values.
   d. Single Index Visualization – Displays a line chart of the three indices based on a specific single value of n.
3. Output Section (Computation Results & Visualizations)
   a. "Computation Results" Box (Top-Right) – Displays the computed values of p and m, along with the numerical results of the First Zagreb Index, Wiener Index, and Gutman Index after pressing the "Calculate Indices" button.
   b. "Graph Visualization" Section (Middle-Right) – Displays the power graph of the dihedral group after pressing the "Graph Visualization" button.

c. "Indices Visualization" Section (Lower-Middle Right) – Shows a comparative line chart of the three indices after pressing the "Indices Visualization" button.
d. "Single Index Visualization" Section (Bottom-Right) – Shows the line chart of the three indices for a specific value of n after pressing the "Single Index Visualization" button.

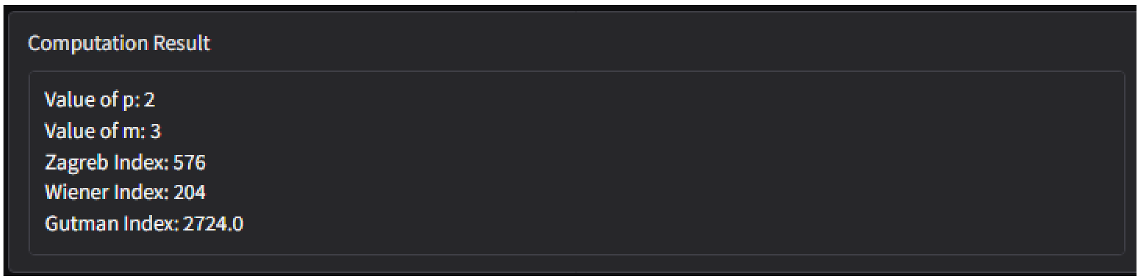

Figure 2.2. Computation Results for $n = 8$

From Figure 2.2, it can be observed that when the input value of n is 8, the resulting values are $p = 2$ and $m = 3$. Subsequently, the computed values for the First Zagreb Index, Wiener Index, and Gutman Index are 576, 204, and 2724, respectively. These results are verified to be accurate, as they are consistent with the values obtained through manual calculation by employing Theorem 1.1 through Theorem 1.3.

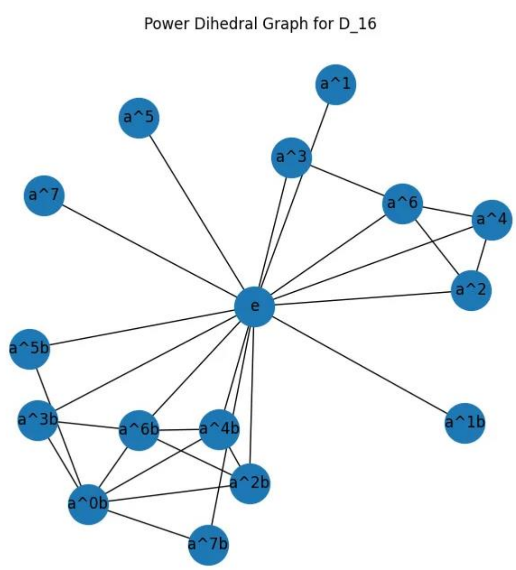

Figure 2.3. Graph Visualization for $n = 8$

Figure 2.3 presents the visualization of the power graph of the dihedral group when $n = 8$. The figure illustrates the power graph of the dihedral group D_{16} , which captures the algebraic structure of the group in terms of power relations among its elements. In this graph, each vertex represents an element of D_{16}, including the identity element e, the rotational elements denoted by powers of a^k, and the reflections represented by elements of the form $a^k b$. An edge is established between two vertices if one is a positive power of the other within the group, thereby encoding the internal power hierarchy of the group elements. As is typical in power graphs of finite groups, the identity element e serves as a central hub, being a power of every other element, and is therefore directly connected to many other vertices. The visual structure of the graph reflects this centrality, with e occupying a prominent, highly connected position. Moreover, the graph naturally decomposes into clusters or subgraphs that reflect the distinct algebraic behavior of rotational and reflectional elements. This graphical representation provides an insightful visualization of the group's internal structure and is particularly useful for analyzing algebraic properties through combinatorial and topological lenses.

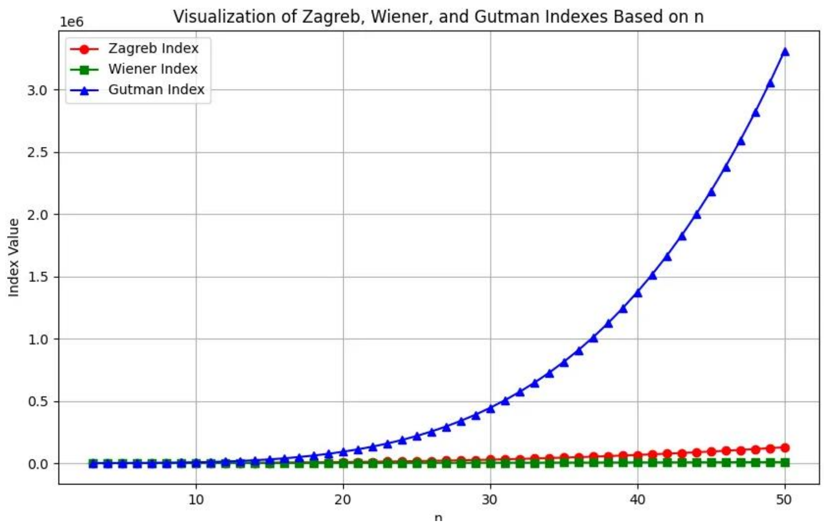

Figure 2.4. Visualization of the Three Index Values Across a Range of n.

Figure 2.4 illustrates the chart of the three Index values over a range of n from 3 to 50. It can be observed that the First Zagreb Index and the Wiener Index have relatively close value ranges, while the Gutman Index shows a significantly larger difference compared to the other two indices. This phenomenon can be attributed to the structural definition of each Index and the underlying algebraic properties of the power graph of the dihedral group D_{2n}. The First Zagreb Index is based solely on the degrees of vertices, while the Wiener Index incorporates shortest path distances between all vertex pairs. In contrast, the Gutman Index combines both the degrees and the distances between vertices

$$Gut(G) = \sum_{\{u,v\} \subseteq V(G)} d(u) \cdot d(v) \cdot dist(u,v) \tag{2.1}$$

Because of this multiplicative combination of degree and distance, the Gutman Index tends to scale faster—especially in graphs with both high-degree vertices and long paths. From an algebraic perspective, the power graph of D_{2n} contains both cyclic subgroups (generated by the rotations a^k) and reflections (of the form $a^k b$). Reflections in D_{2n} typically have order 2 and form many non-trivial power relationships, contributing to the formation of dense subgraphs. This results in certain vertices having high degrees (especially those connected to identity or central elements), while the presence of disconnected or loosely connected components increases the average distance between certain vertex pairs.

As n increases, both the number of group elements and the structural complexity of the graph grow, amplifying the differences between the indices. The Gutman Index becomes particularly sensitive to these changes due to its reliance on both vertex degree and inter-vertex distances. Consequently, the disproportionate growth of the Gutman Index reflects the increased heterogeneity and non-uniform connectivity inherent in the algebraic structure of the dihedral group's power graph.

Table 2.1. Index Values of D_{2n} for $n = 3$ to $n = 17$

No	n	First Zagreb Index	Wiener Index	Gutman Index
1	3	36	24	69
2	4	80	46	202
3	5	150	75	465
4	7	392	154	1645
5	8	576	204	2724
6	9	810	261	4257
7	11	1452	396	9141
8	13	2366	559	17329
9	16	4352	856	38536
10	17	5202	969	48705

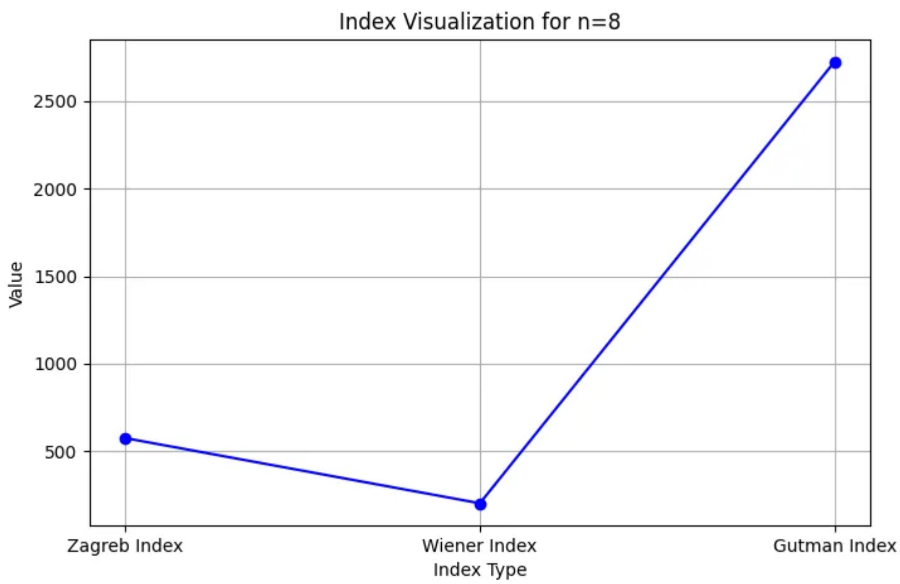

Figure 2.5. Visualization of the Three Index Values for $n = 8$

Figure 2.5. presents the line chart visualization of the three Index values for a specific value of $n = 8$. As previously shown in Figure 2.4., the Gutman Index exhibits a significantly higher value compared to the other two indices. This observation remains valid when focusing on $n = 8$, where the Gutman Index is substantially larger than both the First Zagreb Index and the Wiener Index. This trend becomes increasingly evident as the value of n grows. As clearly illustrated in Table 2.1, the Gutman Index rises at a much faster rate than the First Zagreb and Wiener Indices. For instance, while the First Zagreb Index increases from 36 (at $n = 3$) to 5,202 (at $n = 17$), and the Wiener Index from 24 to 969, the Gutman Index soars from just 69 to a striking 48,705. This sharp escalation highlights that the Gutman Index exhibits a significantly steeper growth pattern compared to the other two indices. From a computational perspective, the algorithmic complexity for calculating the three indices in the power graph of dihedral groups remains constant, i.e., $O(1)$, since all Index computations rely on closed-form mathematical expressions that involve basic arithmetic operations on the parameter n. These formulas eliminate the need for graph traversal or

size-dependent iterations. However, the initial graph construction still requires $O(n^2)$ time due to the nested loop process for generating nodes and identifying power-based edges.

It is important to note, however, that the experimental component of this study remains limited in scope. The investigation focuses primarily on visualizing Index values for specific and relatively small values of n, without delving into broader or asymptotic behavior as $n \to \infty$, nor does it examine structurally distinct cases beyond the $n = p^m$ scenario. As such, while the patterns observed are consistent, they do not yet constitute a comprehensive empirical analysis. Future work could expand on this by exploring larger values of n, incorporating other families of non-abelian groups, or examining the rate of Index growth using normalized or logarithmic scales.

3. CONCLUSION

Based on the results obtained, it can be concluded that by utilizing the Python programming language, this research successfully designed a Python-based computational algorithm to calculate the First Zagreb Index, Wiener Index, and Gutman Index on the power graph of the dihedral group D_{2n} for $n = p^m$. The study also succeeded in visualizing the power graph and generating line charts of the three indices both for specific values of n and across a range of n values.

Beyond the technical implementation, the analysis of the computed indices reveals structural characteristics of the power graph of D_{2n}. For instance, the consistently higher values of the Gutman Index highlight the combined effect of vertex degrees and distances, reflecting the increased complexity and non-uniform connectivity introduced by the reflections and rotations within the group. These findings offer insights into how algebraic properties influence topological invariants in graph representations of non-abelian groups.

Moreover, the development of a Python-based interface not only streamlines the computation but also promotes accessibility for further exploration and educational purposes. The closed-form nature of the formulas ensures efficiency in calculation, while the underlying graph construction allows for structural examination and visualization.

Future work may extend this study by exploring asymptotic behaviors as $n \to \infty$, applying the methodology to other classes of finite groups (e.g., symmetric or alternating groups), or analyzing additional topological indices to further characterize algebraic graph structures. These directions can contribute to broader applications in mathematical chemistry, computational algebra, and theoretical graph theory.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interest regarding the publication of this paper.

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