

The First Zagreb Index and the Narumi-Katayama Index of the Non-Commuting Graph on the Group U_{6n}

Khairatun Hisan¹, Ibrahim Gambo² and I Gede Adhitya Wisnu Wardhana^{3*}

^{1,3}Department of Mathematics Sciences, Faculty of Science, University of Mataram, NTB, Indonesia

²Department of Mathematical Sciences, Faculty of Science, Bauchi State University, Gadau, Nigeria

Email: *adhitya.wardhana@unram.ac.id

Abstract

This paper introduces a novel approach to computing the First Zagreb and Narumi–Katayama indices for non-commuting graphs associated with specific algebraic groups, specifically focusing on the group U_{6n} . The Narumi–Katayama index, first introduced by Narumi and Katayama in 1984, is a degree-based topological index widely used in the study of various graph properties, including its applications in theoretical chemistry. Non-commuting graphs, where two elements are adjacent if and only if they do not commute, have become an intriguing object of study in recent years. To the best of our knowledge, this is the first study to derive closed-form expressions for the First Zagreb and Narumi–Katayama indices on the non-commuting graph of the group U_{6n} . Building on previous research on the detour index and eccentric connectivity in the graph $\Gamma(U_{6n})$, this work makes new contributions by deriving generalized formulas that apply to a broader class of non-commutative groups. Unlike previous studies that focused on commuting or coprime graphs, this research specifically addresses the structure and index computation of non-commuting graphs in a group-theoretic context. The findings offer new theoretical insights into algebraic graph theory by linking degree-based indices with the internal structure of non-abelian groups. These results are expected to expand the understanding of the topological properties of non-commuting graphs and to provide valuable connections to chemical applications.

Keywords: Non-commuting graph; First Zagreb Index; Narumi–Katayama Index; graph topology; group structure.

Abstrak

Artikel ini memperkenalkan pendekatan baru untuk menghitung indeks First Zagreb dan Narumi–Katayama pada graf non-commuting yang terkait dengan grup aljabar tertentu, khususnya berfokus pada grup U_{6n} . Indeks Narumi–Katayama, yang pertama kali diperkenalkan oleh Narumi dan Katayama pada tahun 1984, adalah indeks topologis berbasis derajat yang banyak digunakan dalam studi berbagai properti graf, termasuk penerapannya dalam kimia teoretis. Graf non-commuting, di mana dua elemen saling berhubungan jika dan hanya jika mereka tidak komutatif, telah menjadi objek studi yang menarik dalam beberapa tahun terakhir. Sejauh yang kami ketahui, ini adalah studi pertama yang menghasilkan ekspresi bentuk tertutup untuk indeks First Zagreb dan Narumi–Katayama pada graf non-commuting dari grup U_{6n} . Berdasarkan penelitian sebelumnya tentang indeks detour dan konektivitas eksentrik pada graf $\Gamma(U_{6n})$, karya ini memberikan kontribusi baru dengan menghasilkan rumus umum yang dapat diterapkan pada kelas grup non-komutatif yang lebih luas. Berbeda dengan studi sebelumnya yang berfokus pada graf commuting atau coprime, penelitian ini secara khusus membahas struktur dan perhitungan indeks pada graf non-commuting dalam konteks teori grup. Hasil penelitian ini memberikan wawasan teoretis baru dalam teori graf aljabar dengan menghubungkan indeks berbasis derajat dengan struktur internal grup non-abelian. Diharapkan, temuan ini akan memperluas pemahaman tentang properti topologis graf non-commuting dan memberikan koneksi yang berharga untuk penerapan kimia.

Kata Kunci: Graf non-commuting; Indeks Zagreb Pertama; Indeks Narumi–Katayama; Topologi graf; Struktur grup.

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*) Corresponding author

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1. INTRODUCTION

Graph topological indices are invariant values that remain unchanged for isomorphic graphs and provide insights into the graph's structure. One type of index is the degree-based topological index, widely used in various scientific fields, including chemistry, to analyze the properties of real-world objects such as atoms and molecules. Famous examples of such indices include the Zagreb index, the Narumi–Katayama index, and the total connectivity index [1].

This paper focuses on the First Zagreb Index and the Narumi–Katayama Index. The First Zagreb Index was introduced over four decades ago and is defined as the sum of the squares of the degrees of the vertices in a graph. Previous studies have explored its formula for the total zero-divisor graph of the ring of integers modulo $4p$, conducted by (W) [2]. Meanwhile, the Narumi–Katayama Index was introduced by Narumi and Katayama in 1984. A study by You and Liu determined the minimum value of the Narumi–Katayama Index for bicyclic graphs [3]. Moreover, in 2023, a similar study using a different approach obtained the highest and lowest values of the Narumi–Katayama Index for the set of all bicyclic graphs with n vertices [4]. Another graph-group study can be seen in [5], [6], [7], and [8].

This research will focus on non-commuting graphs, which differ from commuting graphs. In non-commuting graphs, two elements are adjacent if and only if they do not commute. Previous studies have analyzed quaternion groups in various types of graphs, including co-prime, non-co-prime, commuting, non-commuting, and identity graphs [9], [10]. A recent study on the non-commuting graph of U_{6n} calculated the detour index and the eccentric connectivity of $\Gamma(U_{6n})$ [11].

However, despite the numerous studies on various types of non-commuting graphs, no research has specifically developed a general formula for the First Zagreb Index and the Narumi–Katayama Index on the non-commuting graph of the group U_{6n} . This study aims to fill this gap by deriving and analyzing these two topological indices in the context of the non-commuting graph of U_{6n} . The findings are expected to provide new insights into the topological properties of non-commuting graphs and contribute to the understanding of chemical bonds and their theoretical aspects.

2. DEFINITIONS

2.1. First Zagreb Index

One of the fundamental concepts in graph theory is the study of topological indices, which provide structural insights into graphs. These indices play a crucial role in various applications, including mathematical chemistry and network analysis. Among the degree-based topological indices, the First Zagreb Index is widely recognized for its significance in quantifying molecular branching and structural properties of graphs. This index was introduced over four decades ago and has since been applied in numerous studies related to graph invariants [12].

In the context of non-commuting graphs, the First Zagreb Index helps characterize the degree distribution by summing the squares of the degrees of all vertices in the graph. This provides a measure of the overall connectivity and complexity of the underlying structure. To formally define this concept, we present the following definition.

Definition 1. [13] Let K be a graph with the set of vertices $P(K)$ and the set of edges $S(K)$. The First Zagreb Index is defined as follows:

$$M_1(K) = \sum_{p \in P(K)} \text{degree}(p)^2. \quad (1)$$

Example 1. Observe the graph H containing the set $P = \{v_1, v_2, v_3, v_4, v_5\}$ as shown in Figure 1. The following is obtained: $\text{degree}(v_1) = 4$, $\text{degree}(v_2) = 1$, $\text{degree}(v_3) = 1$, $\text{degree}(v_4) = 1$, and $\text{degree}(v_5) = 1$. Next, the value of the first Zagreb index is calculated as follows:

$$\begin{aligned} M_1(H) &= \sum_{v \in P(H)} \text{degree}(v)^2 \\ &= \text{degree}(v_1)^2 + \text{degree}(v_2)^2 + \text{degree}(v_3)^2 + \text{degree}(v_4)^2 + \text{degree}(v_5)^2 \\ &= 4^2 + 1^2 + 1^2 + 1^2 + 1^2 = 20. \end{aligned}$$

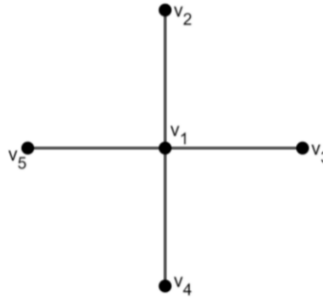


Figure 1. Graph H for Example 1

2.2. Narumi–Katayama Index

The Narumi–Katayama Index is another important degree-based topological index used to analyze graph structures. It is defined as the product of the degrees of all vertices in a graph, providing insights into the connectivity and distribution of vertex degrees. The formal definition is given below.

Definition 2. [1] Let K as a graph with the set of vertices $P(K)$ and the set of edges $S(K)$. The Narumi–Katayama Index commonly denoted as NK , is defined as follows for a graph K :

$$NK(K) = \prod_{p \in P(K)} \text{degree}(p). \quad (2)$$

Example 2. Observe the graph H containing the set $P = \{v_1, v_2, v_3, v_4, v_5\}$ as shown in Figure 2.

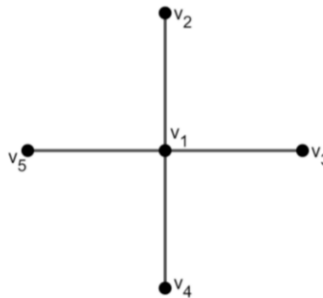


Figure 2. Graph H for Example 2

The following is obtained: $\text{degree}(v_1) = 4$, $\text{degree}(v_2) = 1$, $\text{degree}(v_3) = 1$, $\text{degree}(v_4) = 1$, and $\text{degree}(v_5) = 1$. Next, the value of the Narumi-Katayama index is calculated as follows:

$$\begin{aligned} NK(H) &= \prod_{v \in P(H)} \text{degree}(v) \\ &= \text{degree}(v_1) \cdot \text{degree}(v_2) \cdot \text{degree}(v_3) \cdot \text{degree}(v_4) \cdot \text{degree}(v_5) \\ &= 4 \cdot 1 \cdot 1 \cdot 1 \cdot 1 = 4. \end{aligned}$$

2.3. Non-commuting graph

The non-commuting graph of a group represents the relationships between elements that do not commute. This structure helps in understanding the algebraic properties of the group through graph theory. The formal definition is given below.

Definition 3. [14] Let K be a non-commutative graph, and let $Z(K) = \{p \in K \mid pq = qp \forall q \in K\}$ be the center of K . The non-commuting graph is the complement of the graph $C(K, X)$, where the vertices are the set $K \setminus Z(K)$, and two vertices p and q are adjacent if and only if $pq \neq qp$. It is denoted as graph $C(K, X)$, where $X = K \setminus Z(K)$.

2.4. Group U_{6n}

The group U_{6n} is a specific algebraic structure whose properties influence the characteristics of its associated non-commuting graph. To analyze its structure, we first define the group as follows.

Definition 4. [11] The group U_{6n} , with order $6n$, is defined as $U_{6n} = \langle e, f \mid e^{2n} = f^3 = 1, e^{-1}fe = f^{-1} \rangle$, where U_{6n} for $n \geq 1$ has the center $Z(U_{6n}) = \langle e^2 \rangle$.

Lemma 1. [11] Let $n \geq 1$ be an integer, and let $\Gamma = \Gamma(U_{6n})$. Then, for $0 \leq r \leq n - 1$ and $k = 1, 2$, we have:

$$\text{Degree}(e^{2r+1}) = 4n, \text{ Degree}(e^{2r+1}f^k) = 4n, \text{ and Degree}(e^{2r}f^k) = 3n.$$

3. RESULTS

This study focuses on research discussing the First Zagreb Index and the Narumi-Katayama Index. From the lemma regarding the group U_{6n} mentioned earlier, general properties can be derived. These results are presented in Theorem 1 as follows.

Theorem 1. Let $n \geq 1$ be a positive integer. Consider the non-commuting graph associated with the group U_{6n} . Then, for all r such that $0 \leq r \leq n - 1$, and for $k = 1, 2$, the following holds:

- 1) The degree of (e^{2r+1}) appears n times,
- 2) The degree of $(e^{2r+1}f^k)$ appears $2n$ times,
- 3) The degree of $(e^{2r}f^k)$ appears $2n$ times.

Proof.

A set is constructed containing $r \in \{0, 1, 2, \dots, n-1\}$ where $a = 0$, $b = 1$, and $U_x = n-1$. Explanation: a represents the first term, b represents the difference, and U_x represents the x -th term. It will be demonstrated that for $0 \leq r \leq n-1$, there are n values of r , meaning it will be shown that $x = n$. Using the arithmetic sequence formula:

$$\begin{aligned} U_x &= a + (x-1)b \\ n-1 &= 0 + (x-1)1 \\ n-1 &= x-1 \\ n &= x \end{aligned}$$

Since there are n values of r , degree e^{2r+1} appears n times. Knowing that $k = 1, 2$, it follows that degree $e^{2r+1}f^k$ and degree $e^{2r}f^k$ each appear $2n$ times. ■

From the proof above, general properties regarding the First Zagreb Index and the Narumi-Katayama Index can be derived, with the results presented in Theorems 2 and 3 as follows.

Theorem 2. Assume that there exists a non-commuting graph of the group U_{6n} , where $n \geq 1$. Then, the First Zagreb Index of the non-commuting graph of the group U_{6n} is given by $M_1(U_{6n}) = 66n^3$.

Proof.

From the formula for the First Zagreb Index:

$$M_1(U_{6n}) = \sum_{p \in P(U_{6n})} \text{degree}(p)^2,$$

Where is the set of all vertices in the non-commuting graph of U_{6n} . Based on the structure of the group, the degrees of the vertices are as follows:

1. Degree $(e^{2r+1}) = 4n$, appearing n times,
2. Degree $(e^{2r+1}f^k) = 4n$, appearing $2n$ times,
3. Degree $(e^{2r}f^k) = 3n$, appearing $2n$ times.

Therefore, the index is:

$$\begin{aligned} M_1(U_{6n}) &= \sum_{p \in P(U_{6n})} (\text{degree}(e^{2r+1})^2 + \text{degree}(e^{2r+1}f^k)^2 + \text{degree}(e^{2r}f^k)^2) \\ M_1(U_{6n}) &= n(4n)^2 + 2n(4n)^2 + 2n(3n)^2 \\ M_1(U_{6n}) &= 16n^3 + 32n^3 + 18n^3 \\ M_1(U_{6n}) &= 66n^3. \end{aligned}$$

■

To provide a visual representation of the results, Figure 3 presents the graph of the first Zagreb index (M_1) of the non-commuting graph of the group U_{6n} with respect to different values of n . The graph illustrates that the value of the first Zagreb index increases as n grows, thereby showing the trend of its growth.

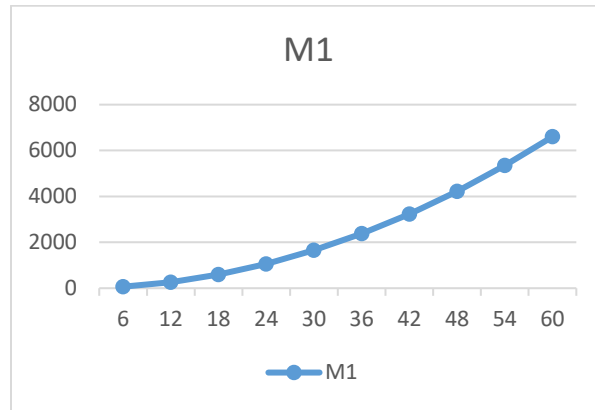


Figure 3. The values of the First Zagreb Index

After obtaining the first Zagreb index theorem for the non-commuting graph of the group U_{6n} , an example case is presented for a simple value of n .

Example 3. Given a non-commuting graph of the group U_{6n} with $n = 3$. Calculate the first Zagreb index of the non-commuting graph of the group U_{6n} .

For $n = 3$, the group U_{6n} is:

$$U_{6n} = \{1, e, e^2, e^3, e^4, e^5, f, ef, e^2f, e^3f, e^4f, e^5f, f^2, ef^2, e^2f^2, e^3f^2, e^4f^2, e^5f^2\}.$$

The first Zagreb index is:

$$M_1(U_{6n}) = \sum_{p \in P(U_{6n})} \text{degree}(p)^2 = 66n^3 = 66(n)^3 = 1782.$$

After proving the first Zagreb index theorem for the non-commuting graph of the group U_{6n} , proceed with the proof for the Narumi-Katayama index, still using the same graph as follows:

Theorem 3. Assume that there a non-commuting graph of the group U_{6n} , where $n \geq 1$. Then, the Narumi-Katayama Index of the non-commuting graph of the group U_{6n} is given by $NK(U_{6n}) = (4n)^{3n} \cdot (3n)^{2n}$.

Proof.

From the formula for the Narumi-Katayama Index:

$$NK(U_{6n}) = \prod_{p \in P(U_{6n})} \text{degree}(p),$$

Where is the set of all vertices in the non-commuting graph of U_{6n} . Based on the structure of the group, the degrees of the vertices are as follows:

- 1) Degree $(e^{2r+1}) = 4n$, appearing n times,
- 2) Degree $(e^{2r+1}f^k) = 4n$, appearing $2n$ times,
- 3) Degree $(e^{2r}f^k) = 3n$, appearing $2n$ times.

Therefore, the index is:

$$NK(U_{6n}) = \prod_{p \in P(U_{6n})} \text{degree}(e^{2r+1}) \cdot \text{degree}(e^{2r+1}f^k) \cdot \text{degree}(e^{2r}f^k)$$

$$NK(U_{6n}) = (4n)^n \cdot (4n)^{2n} \cdot (3n)^{2n}$$

$$NK(U_{6n}) = (4n)^{3n} \cdot (3n)^{2n}. \quad \blacksquare$$

To provide a visual representation of the results, Figure 4 presents the graph of the Narumi-Katayama index (M_1) of the non-commuting graph of the group U_{6n} with respect to different values of n . The graph illustrates that the value of the Narumi-Katayama index increases as n grows, thereby showing the trend of its growth.

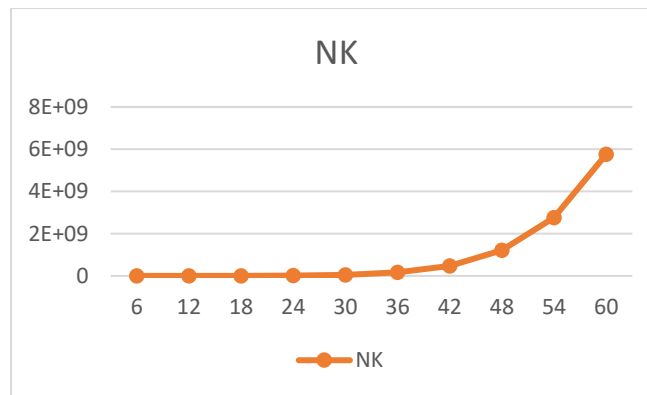


Figure 4. The values of the Narumi-Katayama Index

After obtaining the Narumi-Katayama Index theorem for the non-commuting graph of the group U_{6n} , an example case is presented for a simple value of n .

Example 4. Given a non-commuting graph of the group U_{6n} with $n = 3$. Calculate the Narumi-Katayama Index of the non-commuting graph of the group U_{6n} .

For $n = 3$, the group U_{6n} is:

$$U_{6n} = \{1, e, e^2, e^3, e^4, e^5, f, ef, e^2f, e^3f, e^4f, e^5f, f^2, ef^2, e^2f^2, e^3f^2, e^4f^2, e^5f^2\}.$$

The Narumi-Katayama index is:

$$NK(U_{6n}) = \prod_{p \in P(U_{6n})} \text{degree}(p) = (4n)^{3n} \cdot (3n)^{2n} = (4 \cdot 3)^{3 \cdot 3} \cdot (3 \cdot 3)^{2 \cdot 3} = 274211882898435.$$

A comparison of the First Zagreb Index and the Narumi-Katayama Index of the non-commuting graph of the group U_{6n} is provided in the following table 1 and figure 5. Table 1 illustrates the

computed values of the First Zagreb Index and the Narumi-Katayama Index of the non-commuting graph of the group U_{6n} . The parameters n and $6n$ represent the group's index values, M_1 represent the values of the First Zagreb Index, and NK represent the values of the Narumi-Katayama Index.

Table 1. The numerical values of the First Zagreb Index and the Narumi-Katayama Index for of the non-commuting graph of the group U_{6n} where $n = 1, 2, 3, \dots, 10$.

n	$6n$	M_1	NK
1	6	66	576
2	12	264	73728
3	18	594	1259712
4	24	1056	9437184
5	30	1650	45000000
6	36	2376	161243136
7	42	3234	474360768
8	48	4224	1207959552
9	54	5346	2754990144
10	60	6600	5760000000

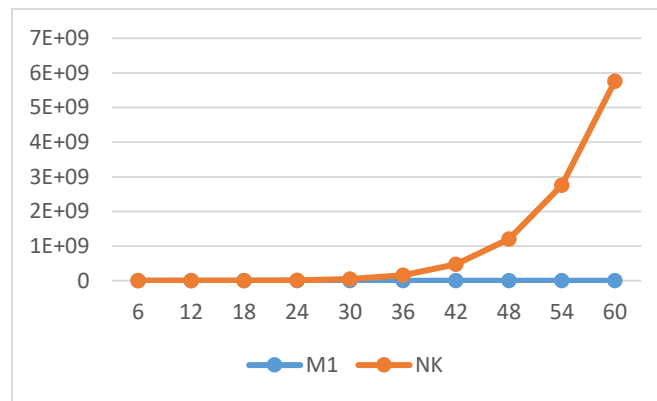


Figure 5. The values of the First Zagreb Index and the Narumi-Katayama Index

As can be seen from the Figure 5, the calculation results of the Narumi-Katayama Index increase more significantly compared to the First Zagreb Index. The calculation of the First Zagreb Index and the Narumi-Katayama Index has been widely studied in molecular graph theory and combinatorial chemistry, but their application in algebraic graph theory remains relatively unexplored.

4. DISCUSSION

4.1. Revised Discussion

This study investigates the First Zagreb Index and the Narumi-Katayama Index of the non-commuting graph on the group U_{6n} , contributing to a broader understanding of algebraic graph theory and its applications in group theory. The results reveal specific structural properties of the non-commuting graph associated with the unit group modulo $6n$, highlighting how graph-based indices can reflect the algebraic characteristics of the underlying group. The primary objective was to

determine explicit formulas for both the First Zagreb Index and the Narumi–Katayama Index of the non-commuting graph of U_{6n} , and analyze their mathematical significance. These indices serve as indicators of the complexity and connectivity of the graph structure, providing insight into vertex interactions based on commutativity in the group. As n increases, the growth behavior of these indices follows a predictable polynomial trend, aligning with findings in earlier studies on graph invariants for similar algebraic structures (e.g., [1], [2], [15]). When comparing the results with previous work on non-commuting graphs of groups such as $\mathbb{Z}_n^*$, dihedral groups, or quaternion groups [16], [17], [18] it becomes evident that the group U_{6n} exhibits a distinct degree distribution. Specifically, the Narumi–Katayama Index grows at a significantly faster rate than the First Zagreb Index, indicating a greater sensitivity to the multiplicative structure and interaction density within the group.

4.2. Theoretical Contributions and Implications

Theoretically, this research contributes to the algebraic characterization of group-based graphs by establishing explicit expressions for key topological indices and linking them to group properties. It demonstrates how commutative relations in U_{6n} influence the structure of its non-commuting graph, offering a deeper understanding of the interplay between group theory and graph invariants. Furthermore, the findings suggest that the Narumi–Katayama Index may serve as a stronger discriminator for detecting high-order interaction patterns in non-commuting graphs, particularly when applied to more complex or composite group structures.

4.3. Future Directions

Several avenues for future research are proposed:

- 1) Generalization to unit groups modulo other composite numbers (e.g., U_{10n} , U_{8n}), to explore whether similar growth patterns in the indices are maintained.
- 2) Comparison with commuting graphs and enhanced commuting graphs of the same group, to investigate duality or complementarity in topological behavior.
- 3) Algorithmic development to compute these indices for large n , potentially contributing to computational algebra systems or graph-theoretic software.

5. CONCLUSIONS

The research focuses on analyzing the First Zagreb Index and the Narumi-Katayama Index associated with the non-commuting graph of the group U_{6n} , specifically for cases where $n \geq 1$. These indices provide valuable insights into the structural properties of the graph derived from the algebraic group U_{6n} . The First Zagreb Index, which is a measure of the sum of the squares of the degrees of the vertices in the graph, is calculated to be $66n^3$. On the other hand, the Narumi-Katayama Index, representing the product of the degrees of all vertices in the graph, is expressed in the form $(4n)^{3n} (3n)^{2n}$. Together, these indices illustrate distinct characteristics of the non-commuting graph and contribute to a deeper understanding of its mathematical structure and combinatorial properties.

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