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THE HARARY INDEX AND THE GUTMAN INDEX IN POWER GRAPHS WITHIN GROUPS OF PRIME ORDER IN INTEGER MODULO GROUP

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ABSTRAK

Artikel ini memperkenalkan dan mendefinisikan konsep-konsep penting seperti Indeks Gutman, Indeks Harary, dan graf pangkat untuk grup bilangan bulat. Ini menyoroti kontribusi signifikan dari Syechah dan rekan-rekannya beserta teorema mereka, yang menunjukkan bahwa graf daya dari grup bilangan bulat menjadi graf lengkap ketika ordernya adalah bilangan prima. Beberapa hasil yang didapatkan adalah rumus umum untuk menghitung Indeks Harary dan Gutman untuk graf pangkat grup bilangan bulat, memberikan wawasan berharga tentang sifat struktural dan keterhubungan antara ilmumatematika dan kimia ini, yang akhirnya menjembatani kesenjangan antara teori matematika dan aplikasi praktis dalam disiplin ilmu ilmiah.
Kata kunci: Indeks Gutman, Indeks Harary, Graf Pangkat

ABSTRACT

This article introduces and defines essential concepts such as the Gutman Index, the Harary Index, and the power graph within the context of integer modulo groups. It highlights Syechah and colleagues' significant contributions and their theorem, demonstrating that the power graph of the integer modulo group becomes a complete graph when the order is prime. Some of the results obtained are general formulas for calculating the Harary and Gutman Indices for the power graph of Integer modulo groups, offering valuable insights into the structural properties and connectivity of these mathematical and chemical compounds, ultimately bridging the gap between mathematical theory and practical applications in scientific disciplines.
Keywords: *Gutman Index, Harary Index, Power Graph*

1. INTRODUCTION

Graph theory, a branch of mathematics, finds applications in various fields, including chemistry. In chemistry, graphs are used to model and analyze molecular structures, making them an invaluable tool in the study of chemical compounds and reactions [1]. Chemists use graph theory to represent atoms as nodes and chemical bonds as edges, allowing for the visualization of complex molecules and the prediction of their properties and behaviors[2]. This approach is crucial in drug discovery, materials science, and understanding the structure-activity relationships in chemical compounds. The application of graph theory in chemistry has revolutionized the way chemists design molecules and study their interactions, leading to significant advancements in the field [3].

Various research studies related to power graphs have explored their applications and properties. Power graphs, which involve constructing vertices based on the powers of elements in a group, have found use in network analysis, social network modeling, and complex systems. Researchers have investigated their role in community detection, where power graphs help identify substructures or clusters within large networks. Additionally, power graphs have been employed in computational biology to analyze protein-protein interaction networks, revealing essential insights into molecular interactions. These research efforts showcase the versatility of power graphs in addressing diverse problems and highlight their potential impact on fields like computer science, biology, and social sciences [4].

Chemical Topological Graphs are fundamental in the field of chemoinformatics, serving as crucial tools for representing molecular structures. Various graph indices, such as the Weiner Index, The Gutman Index, the Zagreb Index, the Harary Index, and the Harmonic Index, have been developed to quantify specific structural features of molecules in many study [5], [6], [7], [8], [9], [10], [11], [12], [13], [14], [15], [16], [17], [18], [19], [20], [21], [22]. These indices find diverse applications in chemistry and computational biology, aiding in drug discovery, chemical property prediction, and the study of molecular properties. They provide valuable insights into the topological characteristics of chemical compounds, contributing significantly to advancements in the field. In previous studies, Syechah et al. delved into the topic of graphs in integer modulo arithmetic [23], while Devandra provided calculations for the Harary Index in coprime graphs within integer modulo arithmetic [14]. However, there has been a noticeable gap in the literature regarding the Harary Index and Gutman Index in power graphs of integer modulo arithmetic. Consequently, this article aims to address this gap by presenting the Harary Index and Gutman Index for power graphs within the framework of integer modulo arithmetic groups.

2. RESEARCH METHOD

The research methodology begins with an extensive literature review to establish a foundation in the field of power graphs. Subsequently, a series of case studies are conducted, considering various orders of power graphs to analyze their properties and characteristics. From these case studies, hypotheses are formulated, postulating certain patterns or relationships within the power graphs. These hypotheses are then rigorously tested and verified through mathematical analysis and computational experiments, employing tools and techniques from graph theory and combinatorics. Finally, the hypotheses that are successfully substantiated through empirical evidence and mathematical proof are elevated to the status of theorems, contributing to the body of knowledge in power graph theory and offering valuable insights into the structural properties of these graphs at different orders.

3. MAIN RESULT

In this article, we commence with an essential introductory section aimed at establishing fundamental terminology and definitions. This initial segment serves as a vital foundation for comprehending and navigating the extensive discussions and analyses that follow. By elucidating key concepts and terminologies, we ensure that readers are equipped with the requisite knowledge to engage effectively with the substantive content presented herein. This groundwork not only enhances clarity but also facilitates a deeper understanding of the subject matter under examination, laying the groundwork for the comprehensive exploration that lies ahead.

Definition 3.1. [14] *The group of integers modulo n is a finite set $\{0,1,2,3,\dots,n-1\}$ equipped with the modulo integer operation. This group is denoted as $\mathbb{Z}_n$.*

In the realm of integer modulo arithmetic, a power graph is a graphical representation where the set of vertice encompasses all members of the group, and two vertices are considered adjacent if one node can be expressed as a power of the other

Definition 3.2. [24] *Let G be a group, a power graph of G, denoted by Γ_G is a graph with all the vertices is G and $x, y \in \Gamma_G$ are adjacent if and only if $x = y^k$ or $y = x^m$ for some $k, m \in \mathbb{N}$.*

In order to define the Harary Index, it is essential to first comprehend the distance between two nodes within a graph.

Definition 3.3. [25] The distance between two vertices x and y in a graph is the shortest path connecting vertice x and vertice y.

The Harary Index, named after the American mathematician Frank Harary in 1969, is a graph theoretical concept. This index plays a significant role in various fields of graph theory and has found applications in diverse scientific disciplines. The Harary Index is defined as follows:

Definition 3.4. [14] Let Γ be a simple connected graph; the Harary Index of Γ is defined as follows:

$$H(\Gamma) = \sum_{u,v \in \Gamma} \frac{1}{d(u,v)}$$

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The Gutman Index, named after the renowned mathematician Ivan Gutman, is a vital graph invariant used in the field of mathematical chemistry and graph theory. This index serves as a quantitative measure of the molecular structure and connectivity of chemical compounds. Its definition is based on the concept of degree, which represents the number of bonds or connections each atom within a molecule has. The Gutman Index, denoted by $Gut(G)$, is calculated by summing the square root of the degrees of all the vertices in a graph. This unique measure provides valuable insights into the complexity and topological properties of molecular structures, making it a valuable tool in chemical and mathematical research.

Definition 3.5. Let Γ be a simple connected graph; the Gutman Index of Γ is defined as follows:

$$Gut(\Gamma) = \sum_{u,v\in\Gamma} deg(u)\, deg(v)\, d(u,v)$$

Syechah and his colleagues have made significant contributions in the discovery of various topological indices of a graph. Their findings, particularly in the context of integer modulo arithmetic groups of order n, have revealed that the power graph is a complete graph if n is a prime number.

Theorem 3.6. [23] *Suppose we have the integer modulo group $\mathbb{Z}_n$. If n is a prime number, then the power graph of $\mathbb{Z}_n$ is a complete graph K_n.*
PROOF. Let n be a prime number, and let $x, y \in \mathbb{Z}_n$ be arbitrary elements. Since x and y are both less than n, and n is a prime number, then $(x,n) = (y,n) = 1$. In other words, x and y are coprime to n. Therefore, there exist $k_1, k_2, m_1, m_2 \in \mathbb{Z}$ such that $k_1x + k_2n = 1$ and $m_1y + m_2n = 1$. Since the group operation is modulo addition in $\mathbb{Z}_n$, it follows that $k_1x = m_1y = 1$, or in other words, $x^{k_1} = y^{m_1} = 1$. Consequently, x and y are also generators of the group, or $\langle x\rangle = \langle y\rangle = \langle 1\rangle = \mathbb{Z}_n$, which implies that $x = y^c$ for some $c \in \mathbb{N}$. As x and y were chosen arbitrarily, this implies that any two elements in the group are adjacent, leading to the conclusion that the prime graph of the group $\mathbb{Z}_n$ is a complete graph K_n. □

Now we can calculate the Harary Index for the power graph of the integer modulo group. This theorem provides a crucial mathematical framework for determining the Harary Index, which is a graph-theoretic measure used to assess the structural properties of power graphs. By applying the theorem's principles to the integer modulo group, we gain valuable insights into the relationships and connectivity patterns among its elements, enhancing our understanding of this fundamental mathematical concept.

Theorem 3.7. *If $n = p^k$ for some $k \in \mathbb{N}$, then the Harary index of the power graph for the integer modulo $\mathbb{Z}_n$ is*

$$H(\Gamma_{\mathbb{Z}_n}) = p^k$$

PROOF. Let n be a prime number, and let $x, y \in \mathbb{Z}_n$, according to Theorem 3.6, we have $d(x,y) = 1$ since the power graph is complete. Given that $\Gamma_{\mathbb{Z}_n}$ has p^k vertices, we have

$$\begin{aligned} H(\Gamma_{\mathbb{Z}_n}) &= \sum_{u,v\in\Gamma} \frac{1}{d(u,v)} \\ &= \sum_{u,v\in\Gamma} \frac{1}{1} \\ &= p^k. \ \square \end{aligned}$$

Now, the Gutman Index will be calculated using the theorem provided by Syechah and colleagues. The Gutman Index is a highly useful graph parameter in the study of mathematical chemistry and graph theory. It is employed to measure the structure and connectivity of chemical molecules through mathematical approaches. Its definition is closely related to the concept of degrees, which represent the number of bonds or connections each atom has within a molecule.

Theorem 3.8. *If $n = p^k$ for some $k \in \mathbb{N}$, then the Gutman index of the power graph for the integer modulo $\mathbb{Z}_n$ is*

$$Gut(\Gamma_{\mathbb{Z}_n}) = p^{3k}$$

PROOF. Let n be a prime number, and let $x, y \in \mathbb{Z}_n$, according to Theorem 3.6, we have $d(x, y) = 1$ and $d(x) = d(y) = p^k$ since the power graph is complete. Due to the fact that $\Gamma_{\mathbb{Z}_n}$ has p^k vertices, we have

$$Gut(\Gamma_{\mathbb{Z}_n}) = \sum_{u,v\in\Gamma} deg(u)\, deg(v)\, d(u, v)$$
$$= \sum_{u,v\in\Gamma} (p^k)(p^k)(1)$$
$$= \sum_{u,v\in\Gamma} (p^{2k})$$
$$= p^{3k}. \square$$

4. CONCLUTIONS

In conclusion, the exploration of mathematical indices like the Gutman Index and the Harary Index within the realm of Integer Modulo Groups provides valuable insights into the structural properties and relationships among their elements. The Gutman Index, as introduced by Syechah and colleagues, offers a unique perspective on molecular structures, enabling researchers in mathematical chemistry to decipher intricate patterns of connectivity. On the other hand, the Harary Index, a fundamental graph-theoretic measure, allows for a deeper understanding of the interplay among elements within these groups, shedding light on their mathematical properties. Both indices play pivotal roles in advancing our comprehension of Integer Modulo Groups, offering a powerful analytical toolkit for mathematicians, chemists, and researchers across various disciplines. As we continue to explore and apply these indices, their significance in mathematical and scientific pursuits becomes increasingly evident, paving the way for further discoveries and applications in the future.

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