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ON THE TOPOLOGICAL INDICES OF A GENERALIZED GRAPH FAMILY USED IN NUMBER-THEORETIC GRAPH REALIZATIONS

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ABSTRACT. In this paper, we study the topological properties of a generalized graph family, constructed by attaching loops to the vertices of a path graph. This family generalizes several graph structures that are used in the literature for realizing graph degree sequences based on number-theoretic sequences. We derive exact general formulas for various degree-based topological indices, including the first and second Zagreb indices, the Randic index, and the Harmonic index for this general family. As an application, we use these formulas to derive several new or known identities for Fibonacci and Lucas numbers by applying them to the known realizations of Fibonacci and Lucas graphs. Furthermore, we show that the ratio of these indices asymptotically converges to the cube of the Golden Ratio.

Keywords. Topological index, graph realization, Fibonacci graph, Lucas graph, Zagreb index
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1. Introduction

The interplay between Graph Theory and Number Theory has long been a fertile ground for mathematical discovery. One of the fundamental bridges connecting these two fields is the "Graph Realization Problem." In its essence, this problem asks a simple yet profound question: Given a sequence of non-negative integers $S = (d_1, d_2, \ldots, d_n)$, does there exist a simple graph G whose vertex degrees are precisely these numbers? If such a graph exists, the sequence is called "graphic" or "realizable." This problem is foundational in network theory and structural chemistry, as it determines the possible topological structures that can arise from a given set of local constraints (degrees).

The classical criteria for realizability are well-established, most notably by the Havel-Hakimi theorem [8, 9] and the Erdős-Gallai theorem [5]. While these theorems provide algorithmic or algebraic methods for arbitrary sequences, a

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recent and growing trend in the literature focuses on the realization of sequences derived from special number-theoretic series.

Several recent studies have successfully investigated the existence conditions for graphs whose degree sequences consist of n consecutive terms from such special sequences. Yurttas Gunes et al. [7] defined the class of "Fibonacci graphs," proving that a sequence of n consecutive Fibonacci numbers is realizable if and only if specific modular arithmetic conditions (related to modulo 3) are met. Following this, Demirci et al. [4] extended the inquiry to "Lucas graphs," utilizing a novel graph invariant $\Omega(G)$ to determine realizability conditions, again finding patterns governed by modulo 3. More recently, the study was generalized to "Tribonacci graphs" by Demirci and Cangul [3], where the existence conditions were shown to depend on the index of the sequence modulo 4. Recent studies have highlighted the importance of structural descriptors in characterizing specialized graph families, ranging from the analysis of topline graphs of trees [6] to the investigation of Harary spectra and energy in regular structures [12].

A careful examination of these foundational papers reveals a striking methodological pattern. To construct the graphical realizations for these diverse number sequences, the authors consistently employ a specific class of non-simple graphs as building blocks. These structures denoted in the literature as L_q, $B_{r,s}$, $T_{a,b,c}$, and $Q_{a,b,c,d}$ are all formed by attaching varying numbers of loops to the vertices of underlying path graphs (P_1, P_2, P_3, P_4) [4, 7]. While these specific graph structures have proven instrumental in solving the realization problems for Fibonacci, Lucas, and Tribonacci sequences, their own structural and topological properties have not yet been systematically analyzed as a unified family.

This paper aims to fill this gap. We first introduce a generalized graph family, which we denote $P_n(l_1, \ldots, l_n)$, consisting of a path graph P_n where $l_i \geq 0$ loops are attached to the i-th vertex. This general family neatly encapsulates L_q (as the $n = 1$ case), $B_{r,s}$ (as the $n = 2$ case), $T_{a,b,c}$ (as the $n = 3$ case), and $Q_{a,b,c,d}$ (as the $n = 4$ case). The primary objective of this work is to conduct a comprehensive analysis of the topological properties of this general family. Specifically, we establish exact formulas for several prominent structural descriptors, namely the Harmonic and Randic indices, alongside both the first and second Zagreb indices. We also compute the Ω invariant, a parameter used extensively to study the realizability and cyclicness of these graphs [3, 7].

The utility of these general formulas, however, extends beyond a simple structural characterization. As a key application, we demonstrate how these topological indices provide a novel method for deriving number-theoretic identities. By substituting the specific parameters from known Fibonacci [7] and Lucas [4] graph realizations into our general index formulas, we establish a direct bridge between the graph topology and the algebraic properties of the number sequences themselves, in some cases confirming known identities and in others revealing new ones.

The structural layout of this study is arranged as follows. We begin in Section 2 by establishing the essential preliminaries, defining the graph families $L_q, B_{r,s}, \ldots,$ and introducing our generalization $P_n(l_i)$. It also recalls the definitions of the topological indices under study. Section 3 presents our main results, beginning with a key lemma on the edge set decomposition of $P_n(l_i)$, followed by our main theorem providing the general formulas for all indices. The specific formulas for the target families are then presented as corollaries. In Section 4, we demonstrate the application of our results by deriving identities for Fibonacci and Lucas numbers. To conclude the study, Section 5 offers a summary of our main contributions and identifies several promising avenues for prospective research.

2. Preliminaries and Definitions

In this section, we introduce the fundamental graph-theoretic notation and definitions used throughout the paper. For any background terms not explicitly detailed in the following sections, we assume the definitions provided in West [13], and Bondy and Murty [1].

A finite undirected graph G is defined by its vertex set $V(G)$ and edge set $E(G)$. We refer to the cardinality of the vertex set as the order of G (denoted by n), while the total number of edges, $|E(G)|$, represents the size of the graph, m. If two vertices $u, v \in V$ are linked by an edge $uv \in E$, they are considered adjacent.

For any vertex v, its degree, symbolized as $d(v)$, represents the total count of edge endpoints incident to v. In the context of graphs with self-loops, it is important to note that each loop adds 2 to the degree of its incident vertex. The resulting set $D = \{d_1, d_2, \ldots, d_n\}$ constitutes the degree sequence of the graph G.

Having established these basic notions, we now review the specific graph structures ($L_q, B_{r,s}, T_{a,b,c}$, and $Q_{a,b,c,d}$) that have been utilized in the literature to construct graph realizations for number-theoretic sequences [3, 4, 7].

2.1. The Target Graph Families ($L_q, B_{r,s}, T_{a,b,c}, Q_{a,b,c,d}$).

As we noted in the introduction, the literature on graph realizations consistently relies on a set of core building blocks [3, 4, 7]. Let's formally introduce the key members of this "family" that motivate our study. All these graphs are non-simple and are constructed by adding loops to the vertices of path graphs.

In this context, we recall that a loop at a vertex v contributes 2 to its degree, $d(v)$.

The L_q family: This is the simplest case, built upon a path graph of a single vertex (P_1). The graph L_q consists of a single vertex v and $q \geq 0$ loops attached to it. Consequently, the degree of the vertex is $d(v) = 2q$ [3].

The $B_{r,s}$ family: This family is built upon a path graph P_2 (a single edge between two vertices, v_1 and v_2). The graph $B_{r,s}$ is formed by adding $r \geq 0$ loops to v_1 and $s \geq 0$ loops to v_2. The degrees of the vertices are therefore $d(v_1) = 2r+1$ and $d(v_2) = 2s + 1$ [7].

The $T_{a,b,c}$ family: This family is built upon a path graph P_3 (with vertices v_1, v_2, v_3 and edges v_1v_2, v_2v_3). The graph $T_{a,b,c}$ is formed by adding $a \geq 0$ loops to the first vertex v_1, $b \geq 0$ loops to the central vertex v_2, and $c \geq 0$ loops to the third vertex v_3. The resulting degrees are $d(v_1) = 2a + 1$, $d(v_2) = 2b + 2$, and $d(v_3) = 2c + 1$ [3].

The $Q_{a,b,c,d}$ family: Following the same pattern, this family is built upon a path graph P_4 (with vertices v_1, v_2, v_3, v_4). The graph $Q_{a,b,c,d}$ is formed by adding

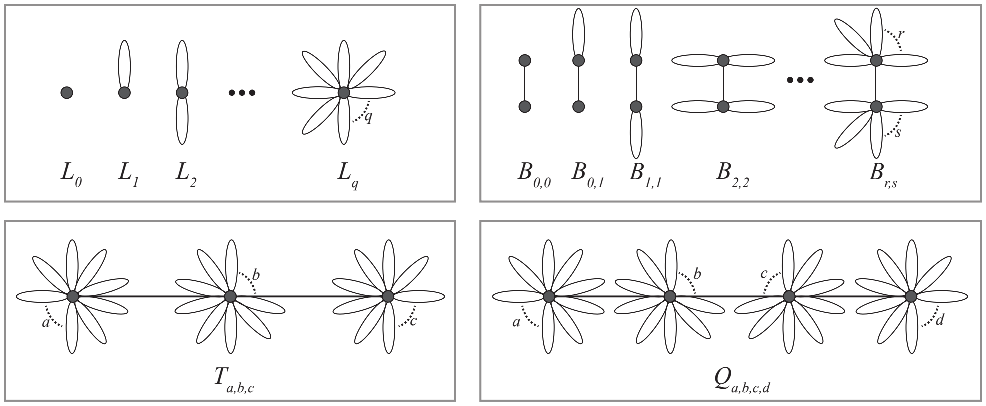

FIGURE 1. Visual representation of the target graph families: L_q, $B_{r,s}$, $T_{a,b,c}$, and $Q_{a,b,c,d}$.

a, b, c, d loops to the vertices v_1, v_2, v_3, v_4, respectively. The degrees are $d(v_1) = 2a + 1$, $d(v_2) = 2b + 2$, $d(v_3) = 2c + 2$, and $d(v_4) = 2d + 1$ [3].

A visual representation of these four graph families is presented in Figure 1. As one can observe, these four distinct families are not truly "distinct" at all; they are specific instances of a single, unified construction: attaching loops to the vertices of a path graph P_n for $n = 1, 2, 3$, and 4. This clear, underlying pattern motivates us to define a general family that encapsulates all of them, which we will introduce in the following section.

2.2. **A Generalization: The $P_n(l_i)$ Family.** Based on the common structure observed in Section 2.1, we now formalize and generalize this "path-with-loops" construction. This allows us to unify all four target families under a single, comprehensive framework.

Definition 2.1 (The $P_n(l_i)$ Family)**.** Let $n \geq 1$ be an integer and let $l_1, l_2, \ldots, l_n$ be non-negative integers. We define the generalized graph $G = P_n(l_1, \ldots, l_n)$ as follows:

If $n = 1$, G consists of a single vertex v_1 with l_1 loops attached. The degree of the vertex is $d(v_1) = 2l_1$.

If $n \geq 2$, G is constructed from a path graph P_n on vertices $v_1, \ldots, v_n$ by adding l_i loops to each corresponding vertex v_i for $i = 1, \ldots, n$.

The degrees of the vertices for $n \geq 2$ are derived from the degrees of the path graph P_n (which are $1, 2, \ldots, 2, 1$) and the $2l_i$ contributions from the loops at each vertex v_i. This results in:

$$d(v_i) = \begin{cases} 2l_1 + 1 & \text{if } i = 1 \\ 2l_i + 2 & \text{if } 1 < i < n \\ 2l_n + 1 & \text{if } i = n \end{cases}.$$

Note that for the $n = 2$ case, this formula simplifies to $d(v_1) = 2l_1 + 1$ and $d(v_2) = 2l_2 + 1$, matching the structure of $B_{r,s}$. Similarly, the definitions for $n = 3$ and $n = 4$ precisely match the structures of $T_{a,b,c}$ and $Q_{a,b,c,d}$, respectively.

The number of vertices in G is $n(G) = n$. The total number of edges (the size) is $m(G) = l_1$ if $n = 1$, and $m(G) = (n-1) + \sum_{i=1}^{n} l_i$ if $n \geq 2$.

2.3. **Definitions of Topological Indices.** In the field of chemical graph theory, a topological index (TI) can be thought of as a "fingerprint" for a graph's structure. It is a single numerical value, formally known as a graph invariant, which means it doesn't change no matter how we label the vertices of the graph. These indices are powerful tools because they allow us to correlate a graph's structure (like its size, shape, or branching) with its physical or chemical properties (like stability, boiling point, or energy).

Since our generalized graph family $P_n(l_i)$ contains loops, we must first establish our methodology. Our approach follows the standard method established in the literature [3, 4, 7], where a loop at a vertex v is regarded as an edge incident to v twice, such that each loop contributes 2 to the total degree $d(v)$.

Given a graph $G = (V, E)$, with vertex degrees $d(v)$ for $v \in V$, we will investigate the following well-established topological indices:

(1) *The Zagreb Indices (M_1, M_2):* These are among the oldest and most-studied indices. M_1 is often described as the "total energy" of the graph, while M_2 quantifies the energy of the bonds (edges).

$$M_1(G) = \sum_{v \in V(G)} d(v)^2 \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d(u)d(v).$$

The Zagreb indices are among the most established degree-based descriptors in the literature. Related investigations have also examined associated invariants, such as the properties of Zagreb coindices under various graph operations [10].

(2) *The Randić (Connectivity) Index (R):* Perhaps the most famous TI, the Randić index is a fundamental measure of molecular branching.

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

(3) *The Harmonic (H) Index:* This index is closely related to the Randić index and is another effective measure of graph branching.

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

(4) *The Ω (Omega) Invariant:* Finally, we include the Ω invariant. This is not a classical TI, but rather a powerful, more recent graph invariant introduced by Delen and Cangul in [2]. It is the primary analytical tool used in the very papers that motivate our study [3, 7].

What makes it so useful? It was originally defined based only on the degree sequence of a graph, $D = \{1^{(a_1)}, 2^{(a_2)}, \ldots, \Delta^{(a_\Delta)}\}$, as:

$$\Omega(G) = \sum_{i=1}^{\Delta} (i-2)a_i.$$

The authors then proved that this value is elegantly connected to the graph's most basic parameters: Size m and order n [2, Theorem 2.1]. This key theorem states:

$$\Omega(G) = 2(m-n).$$

This invariant's true power, and the reason it is so relevant to our work, is its direct relationship with the number of "faces" or "closed regions" r in the graph, which includes the loops we are studying [2, Corollary 3.1]. For our calculations, we will use the practical $2(m-n)$ formulation.

3. Main Results: Topological Indices of the $P_n(l_i)$ Family

We now arrive at the core computational results of this paper. In this section, we will derive the general formulas for the topological indices of the $P_n(l_i)$ family, as defined in Section 2.2.

To compute the edge-based indices (such as M_2, R, and H), we must first analyze the contributions from all edges in the graph. As is clear from its definition, the edge set of $P_n(l_i)$ can be naturally partitioned into two distinct types: the "path edges" and the "loop edges". We formalize this fundamental decomposition in the following lemma, which will serve as the foundation for our main theorem.

Lemma 3.1. *The degree sequence of the graph $G = P_n(l_1, \ldots, l_n)$ is $\{2.l_1 + 1, 2.l_2 + 2, ..., 2.l_{n-1} + 2, 2.l_n + 1\}$.*

Lemma 3.2. *Let $G = P_n(l_1, \ldots, l_n)$. The edge set $E(G)$ can be partitioned into two disjoint sets: the set of path edges E_{path} and the set of loop edges E_{loop}, where*

$$E_{path} = \{v_1v_2, v_2v_3, ..., v_{i-1}v_i, ..., v_{n-1}v_n\}$$

$$E_{loop} = \{(v_1v_1)^{(l_1)}, (v_2v_2)^{(l_2)}, ..., (v_iv_i)^{(l_i)}, ..., (v_{n-1}v_{n-1})^{(l_{n-1})}, (v_nv_n)^{(l_n)}\}.$$

Theorem 3.3. *Let $G = P_n(l_1, \ldots, l_n)$. The first and second Zagreb indices of G are given as follows:*

(1)

$$M_1(G) = \begin{cases} 4l_1^2 & \text{if } n = 1 \\ 4\sum_{i=1}^{n} l_i^2 + 4l_1 + 4l_n + 8\sum_{i=2}^{n-1} l_i + 4n - 6 & \text{if } n \geq 2 \end{cases}.$$

(2)

$$M_2(G) = M_{2,loop}(G) + M_{2,path}(G).$$

The contribution from the loop edges (E_{loop}) is:

$$M_{2,loop}(G) = \begin{cases} 4l_1^3 & \text{if } n = 1 \\ (4l_1^3 + 4l_1^2 + l_1) + (4l_n^3 + 4l_n^2 + l_n) + \sum_{i=2}^{n-1}(4l_i^3 + 8l_i^2 + 4l_i) & \text{if } n \geq 2 \end{cases}.$$

The contribution from the path edges (E_{path}) is:

$$M_{2,path}(G) = \begin{cases} 0 & \text{if } n = 1 \\ 4l_1l_2 + 2l_1 + 2l_2 + 1 & \text{if } n = 2 \\ (4l_1l_2 + 4l_1 + 2l_2 + 2) + (4l_2l_3 + 2l_2 + 4l_3 + 2) & \text{if } n = 3 \\ (4l_1l_2 + 4l_1 + 2l_2 + 2) + \sum_{i=2}^{n-2}(4l_il_{i+1} + 4l_i + 4l_{i+1} + 4) & \\ \quad +(4l_{n-1}l_n + 2l_{n-1} + 4l_n + 2) & \text{if } n \geq 4 \end{cases}.$$

Proof. We will prove each item of the theorem by direct calculation, using the vertex degrees from Lemma 3.1 and the edge set decomposition from Lemma 3.2.

1. By definition, $M_1(G) = \sum_{i=1}^{n} d(v_i)^2$. We proceed by cases.

Case $n = 1$: $G = L_{l_1}$ has one vertex v_1 with $d(v_1) = 2l_1$. Thus, $M_1(G) = (2l_1)^2 = 4l_1^2$.

Case $n \geq 2$: We partition the sum based on the three types of vertex degrees (two endpoints, $n-2$ middle points):

$$M_1(G) = d(v_1)^2 + d(v_n)^2 + \sum_{i=2}^{n-1} d(v_i)^2.$$

Substituting the degree formulas from Definition 2.1:

$$M_1(G) = (2l_1 + 1)^2 + (2l_n + 1)^2 + \sum_{i=2}^{n-1}(2l_i + 2)^2.$$

Expanding the terms:

$$M_1(G) = (4l_1^2 + 4l_1 + 1) + (4l_n^2 + 4l_n + 1) + \sum_{i=2}^{n-1}(4l_i^2 + 8l_i + 4).$$

Collecting the terms by their powers of l_i and the constant terms:

$$M_1(G) = \left(4\sum_{i=1}^{n} l_i^2\right) + \left(4l_1 + 4l_n + 8\sum_{i=2}^{n-1} l_i\right) + \left(1 + 1 + \sum_{i=2}^{n-1} 4\right).$$

Simplifying the sum of constants:

$$M_1(G) = 4\sum_{i=1}^{n} l_i^2 + 4l_1 + 4l_n + 8\sum_{i=2}^{n-1} l_i + (2 + 4(n-2)).$$

$$M_1(G) = 4\sum_{i=1}^{n} l_i^2 + 4l_1 + 4l_n + 8\sum_{i=2}^{n-1} l_i + 4n - 6.$$

This completes the proof for $M_1(G)$.

2. A loop v_iv_i contributes $d(v_i)d(v_i) = d(v_i)^2$. Since there are l_i loops at vertex v_i, the total loop contribution is $M_{2,\text{loop}}(G) = \sum_{i=1}^{n} l_i d(v_i)^2$. For $n = 1$, this is $l_1(2l_1)^2 = 4l_1^3$. For $n \geq 2$, we partition the sum as we did for $M_1(G)$:

$$M_{2,\text{loop}}(G) = l_1 d(v_1)^2 + l_n d(v_n)^2 + \sum_{i=2}^{n-1} l_i d(v_i)^2.$$

$$= l_1(2l_1+1)^2 + l_n(2l_n+1)^2 + \sum_{i=2}^{n-1} l_i(2l_i+2)^2.$$

Expanding this yields the formula for $M_{2,\text{loop}}(G)$ as stated in the theorem.

The sum over the $n-1$ path edges, $\sum_{i=1}^{n-1} d(v_i)d(v_{i+1})$. We prove this by the cases defined in the theorem. For $n=1$, the sum is empty, so $M_{2,\text{path}}(G)=0$. For $n=2$, the sum has one term: $d(v_1)d(v_2)=(2l_1+1)(2l_2+1)$, which expands to $4l_1l_2+2l_1+2l_2+1$. For $n\geq 3$, the sum $d(v_1)d(v_2)+d(v_2)d(v_3)+\dots$ is partitioned according to the degree formulas, which directly yields the expressions for the $n=3$ and $n\geq 4$ cases as stated.

□

We now move to the connectivity indices. The following two theorems present the results for the Randić and Harmonic indices. We present the theorems separately for clarity, followed by a unified proof, as their derivation follows an identical methodology based on Lemma 3.2.

Theorem 3.4. *Let $G=P_n(l_1,\dots,l_n)$ for $n\geq 1$. The Randić Index $R(G)$ is given by:*

$$R(G) = R_{loop}(G) + R_{path}(G),$$

where:

(1) *The total contribution from loop edges is:*

$$R_{loop}(G) = \sum_{i=1}^{n} \frac{l_i}{d(v_i)} = \begin{cases} \frac{1}{2} & \text{if } n=1 \\ \frac{l_1}{2l_1+1} + \frac{l_n}{2l_n+1} + \frac{1}{2}\sum_{i=2}^{n-1}\frac{l_i}{l_i+1} & \text{if } n\geq 2 \end{cases}.$$

(2) *The total contribution from path edges is:*

$$R_{path}(G) = \begin{cases} \frac{1}{\sqrt{(2l_1+1)(2l_2+1)}} & \text{if } n=2 \\ \frac{1}{\sqrt{2(2l_1+1)(l_2+1)}} + \frac{1}{\sqrt{2(l_2+1)(2l_3+1)}} & \text{if } n=3 \\ \frac{1}{\sqrt{2(2l_1+1)(l_2+1)}} + \frac{1}{2}\sum_{i=2}^{n-2}\frac{1}{\sqrt{(l_i+1)(l_{i+1}+1)}} + \frac{1}{\sqrt{2(l_{n-1}+1)(2l_n+1)}} & \text{if } n\geq 4 \end{cases}.$$

For the case $n=1$ it is easy to see $R_{path}(G)=0$.

Theorem 3.5. *Let $G=P_n(l_1,\dots,l_n)$ for $n\geq 1$. The Harmonic Index $H(G)$ is given by:*

$$H(G) = H_{loop}(G) + H_{path}(G),$$

where:

(1) *The total contribution from loop edges is:*

$$H_{loop}(G) = \sum_{i=1}^{n} \frac{l_i}{d(v_i)} = \begin{cases} \frac{1}{2} & \text{if } n=1 \text{ (and } l_1>0) \\ \frac{l_1}{2l_1+1} + \frac{l_n}{2l_n+1} + \frac{1}{2}\sum_{i=2}^{n-1}\frac{l_i}{l_i+1} & \text{if } n\geq 2 \end{cases}.$$

(2) *The total contribution from path edges is:*

$$H_{path}(G) = \sum_{i=1}^{n-1} \frac{2}{d(v_i)+d(v_{i+1})},$$

which, for $n \geq 2$, expands to:

$$H_{path}(G) = \begin{cases} \frac{1}{l_1+l_2+1} & \text{if } n = 2 \\ \frac{2}{2l_1+2l_2+3} + \frac{2}{2l_2+2l_3+3} & \text{if } n = 3 \\ \frac{2}{2l_1+2l_2+3} + \sum_{i=2}^{n-2} \frac{1}{l_i+l_{i+1}+2} + \frac{2}{2l_{n-1}+2l_n+3} & \text{if } n \geq 4 \end{cases}.$$

For the case $n = 1$ it is easy to see $H_{path}(G) = 0$.

Proof of Theorems 3.4 and 3.5. The proofs for both indices are analogous and rely on partitioning the total sum into loop and path contributions.
1. Loop Contribution (R_{loop} and H_{loop}): The methodologies for both indices are identical. A loop v_iv_i at vertex v_i contributes $1/d(v_i)$ to both $R(G)$ and $H(G)$, since:

$$\frac{1}{\sqrt{d(v_i)d(v_i)}} = \frac{1}{d(v_i)} \quad \text{and} \quad \frac{2}{d(v_i)+d(v_i)} = \frac{1}{d(v_i)}.$$

Since there are l_i loops at vertex v_i, the total loop contribution for both indices is $H_{\text{loop}}(G) = R_{\text{loop}}(G) = \sum_{i=1}^{n} \frac{l_i}{d(v_i)}$. Substituting the degree definitions and separating the cases for $n = 1$ and $n \geq 2$ yields the formulas stated in the theorems.
2. Path Contribution (R_{path} and H_{path}): The path contribution is calculated by summing over the $n-1$ path edges, using the respective functions for $R(G)$ and $H(G)$. We apply the degree formulas from Definition 2.1 to the path edges v_iv_{i+1} for the cases $n = 2, 3$, and $n \geq 4$. For instance, for $R(G)$ in the $n \geq 4$ case, the middle terms are:

$$\sum_{i=2}^{n-2} \frac{1}{\sqrt{d(v_i)d(v_{i+1})}} = \sum_{i=2}^{n-2} \frac{1}{\sqrt{(2l_i+2)(2l_{i+1}+2)}} = \frac{1}{2}\sum_{i=2}^{n-2} \frac{1}{\sqrt{(l_i+1)(l_{i+1}+1)}}.$$

Analogous substitutions for the other terms and for $H(G)$ yield the formulas stated in Theorems 3.4 and 3.5. ☐

By substituting the specific parameters n and l_i into our general theorems, we obtain the topological indices for the target families L_q, $B_{r,s}$, $T_{a,b,c}$, and $Q_{a,b,c,d}$. This unification is summarized in Table 1 for Zagreb indices and in Table 2 for Randić and Harmonic indices.

TABLE 1. Zagreb indices for specific sub-families of $P_n(l_i)$.

Family	$M_1(G)$	$M_2(G)$
L_q	$4q^2$	$4q^3$
$B_{r,s}$	$4(r^2+s^2+r+s)+2$	$4(r^3+s^3+r^2+s^2+rs)+3(r+s)+1$
$T_{a,b,c}$	$4(a^2+b^2+c^2+a+2b+c)+6$	$4(a^3+c^3+b^3+a^2+c^2+2b^2)$ $+4(ab+bc)+8b+5(a+c)+4$
$Q_{a,b,c,d}$	$4(a^2+b^2+c^2+d^2)$ $+4(a+d)+8(b+c)+10$	$\sum_{i\in\{a,d\}}(4i^3+4i^2+i)+\sum_{j\in\{b,c\}}(4j^3+8j^2+4j)$ $+(4ab+4bc+4cd+4a+6b+6c+4d+8)$

TABLE 2. Randić and Harmonic indices for specific sub-families of $P_n(l_i)$.

Family	$R(G)$	$H(G)$
L_q	$1/2$	$1/2$
$B_{r,s}$	$\frac{4rs+r+s+\sqrt{4rs+2r+2s+1}}{4rs+2r+2s+1}$	$\frac{r}{2r+1}+\frac{s}{2s+1}+\frac{1}{r+s+1}$
$T_{a,b,c}$	$\left(\frac{a}{2a+1}+\frac{b}{2b+2}+\frac{c}{2c+1}\right) + \frac{1}{\sqrt{(2a+1)(2b+2)}}+\frac{1}{\sqrt{(2b+2)(2c+1)}}$	$\left(\frac{a}{2a+1}+\frac{b}{2b+2}+\frac{c}{2c+1}\right) + \frac{2}{2a+2b+3}+\frac{2}{2b+2c+3}$
$Q_{a,b,c,d}$	$\left(\frac{a}{2a+1}+\frac{b}{2b+2}+\frac{c}{2c+2}+\frac{d}{2d+1}\right) + \frac{1}{\sqrt{(2a+1)(2b+2)}}+\frac{1}{2\sqrt{(b+1)(c+1)}}+\frac{1}{\sqrt{(2c+2)(2d+1)}}$	$\left(\frac{a}{2a+1}+\frac{b}{2b+2}+\frac{c}{2c+2}+\frac{d}{2d+1}\right) + \frac{2}{2a+2b+3}+\frac{1}{b+c+2}+\frac{2}{2c+2d+3}$

Having established the general formulas for the classical degree-based topological indices, we now turn our attention to a structural invariant that is central to the literature motivating this study. As discussed in the introduction, the Ω invariant is not merely a numerical value but a direct measure of the "cyclicness" of a graph. The following theorem establishes the precise relationship between our loop parameters l_i and the cyclomatic number of the generalized graph $P_n(l_i)$.

Theorem 3.6. *Let $G = P_n(l_1, \dots, l_n)$ be a connected graph with $n \geq 1$.*

(1) *The Ω invariant of G depends solely on the total number of loops and is given by:*

$$\Omega(G) = 2\left(\sum_{i=1}^{n} l_i - 1\right).$$

(2) *Let r and c denote the cyclomatic number (or the number of fundamental cycles) and number of components of a given graph G respectively. Using the relation $r = \frac{\Omega(G)}{2} + c$ given in [2], with $c = 1$, we determine the number of fundamental cycles as:*

$$r = \sum_{i=1}^{n} l_i.$$

Proof. 1. From the fundamental property of the Omega invariant [2], we know that $\Omega(G) = 2(m-n)$. For the graph $G = P_n(l_1, \dots, l_n)$, the number of vertices is n. The number of edges m consists of $n-1$ edges from the path structure (if $n = 1$, this is 0) plus the total number of loops $\sum l_i$. Thus, $m = (n-1) + \sum_{i=1}^{n} l_i$. Substituting these into the formula:

$$\Omega(G) = 2\left((n - 1 + \sum_{i=1}^{n} l_i) - n\right) = 2\left(\sum_{i=1}^{n} l_i - 1\right).$$

2. Since G is a connected graph, the number of components is $c = 1$. Using the result from [2]:

$$r = \frac{\Omega(G)}{2} + 1 = \frac{2(\sum l_i - 1)}{2} + 1 = (\sum_{i=1}^{n} l_i - 1) + 1 = \sum_{i=1}^{n} l_i.$$

This result confirms that the cyclomatic complexity of graphs in this family is exactly equal to the total number of loops attached to the path vertices. □

Remark 3.7. It is well-known that for any acyclic connected graph (tree), the Ω invariant is −2 [2]. Our generalized formula is consistent with this property. If we set all $l_i = 0$ (meaning no loops are attached), the graph becomes a simple path graph P_n, which is a tree. In this case, our formula gives:

$$\Omega(P_n) = 2(0-1) = -2$$

which aligns perfectly with the established theory.

4. Application: Deriving Number-Theoretic Identities

In this section, we demonstrate the utility of our generalized topological indices by applying them to specific graph realizations of Fibonacci and Lucas numbers found in the literature. We present three distinct types of applications: a ”degree recovery” method for single-vertex graphs ($n = 1$), an establishment of ”cross sequence” for Lucas and Fibonacci numbers ($n = 2$) and a ”geometric identity derivation” for path-like graphs ($n = 3$).

4.1. Degree Recovery in Single-Vertex Graphs ($n = 1$).

Let us consider a specific ratio of topological indices, which we define as $\mathcal{Q}(G)$:

$$\mathcal{Q}(G) = \frac{M_2(G)}{R(G) \cdot M_1(G)}.$$

We show that for the L_q family, this ratio allows us to recover the generating number sequence directly from the topological indices.

Example 4.1. For the Fibonacci graph realization in [7] L_q with parameter $q = F_{3k}/2$, the vertex degree is $d(v) = F_{3k}$. Using our general formulas, we obtain $M_1 = (F_{3k})^2$, $M_2 = (F_{3k})^3/2$. Substituting these values:

$$\mathcal{Q}(L_{F_{3k}/2}) = \frac{(F_{3k})^3/2}{(1/2)\cdot(F_{3k})^2} = F_{3k}.$$

Example 4.2 (Lucas Graph $L_{L_{3k}/2}$)**.** Similarly, consider the Lucas graph realization where the vertex degree corresponds to the Lucas number L_{3k} (i.e., $q = L_{3k}/2$) [4]. Using the same methodology:

$$M_1 = (L_{3k})^2, \quad M_2 = \frac{(L_{3k})^3}{2}, \quad R = \frac{1}{2}$$

The ratio yields:

$$\mathcal{Q}(L_{L_{3k}/2}) = \frac{(L_{3k})^3/2}{(1/2)\cdot(L_{3k})^2} = L_{3k}.$$

Remark 4.3. These examples confirm that for the class of loop-graphs L_q, the topological index ratio $\mathcal{Q}(G)$ acts as a generic “degree recovery operator,” extracting the underlying number-theoretic value (F_{3k} or L_{3k}) solely from the topological descriptors of the graph.

Remark 4.4 (Asymptotic Behavior and the Golden Ratio). The result $\mathcal{Q}(L_{F_{3k}/2}) = F_{3k}$ allows us to bridge graph topology with the asymptotic properties of the Fibonacci sequence. Consider two consecutive graphs in this sequence, G_k generated by F_{3k} and G_{k+1} generated by $F_{3(k+1)} = F_{3k+3}$. The ratio of their recovered topological values is:

$$\frac{\mathcal{Q}(G_{k+1})}{\mathcal{Q}(G_k)} = \frac{F_{3k+3}}{F_{3k}}.$$

It is a well-known property of Fibonacci numbers that $\lim_{n\to\infty} \frac{F_{n+1}}{F_n} = \phi$, where $\phi = \frac{1+\sqrt{5}}{2}$ is the Golden Ratio. Consequently, as the order of the graph increases ($k \to \infty$), the ratio of the topological indices of consecutive graphs converges to the cube of the Golden Ratio:

$$\lim_{k\to\infty} \frac{\mathcal{Q}(G_{k+1})}{\mathcal{Q}(G_k)} = \phi^3 = 2\phi + 1 \approx 4.236.$$

This demonstrates that the proposed topological index ratio $\mathcal{Q}(G)$ not only recovers the integer values of the sequence but also preserves its fundamental asymptotic geometric properties.

4.2. **Identities from $B_{r,s}$ Graphs ($n = 2$).** We calculate the First Zagreb Index for the Lucas graph realization $B_{r,s}$ where the vertex degrees are consecutive Lucas numbers. According to [4], for the degree sequence $\{L_{3k+1}, L_{3k+2}\}$, the loop parameters are $l_1 = (L_{3k+2} - 1)/2$ and $l_2 = (L_{3k+1} - 1)/2$.

From Theorem 3.3, for $n = 2$, $M_1(G) = d(v_1)^2 + d(v_2)^2$. Substituting the Lucas numbers:

$$M_1(B_{r,s}) = L_{3k+2}^2 + L_{3k+1}^2.$$

Using the identity in [11] relating sum of squares of Lucas numbers to Fibonacci numbers, $L_n^2 + L_{n+1}^2 = 5F_{2n+1}$, we derive the following relationship:

$$M_1(B_{r,s}) = 5F_{6k+3}.$$

Remark 4.5. This result is particularly interesting as it establishes a "cross-sequence" bridge. The topological energy (M_1) of a graph constructed purely from Lucas numbers is shown to be directly proportional to a specific Fibonacci number (F_{6k+3}), with a proportionality constant of 5.

4.3. **Geometric Identities from $T_{a,b,c}$ Graphs ($n = 3$).** We now consider the connected realization of consecutive Fibonacci numbers $\{F_{3k+4}, F_{3k+3}, F_{3k+2}\}$ as the graph $T_{a,b,c}$ (or $P_3(a, b, c)$) where $a = \frac{F_{3k+4}-1}{2}$, $b = \frac{F_{3k+3}-2}{2}$ and $c = \frac{F_{3k+2}-1}{2}$ [7]. The degrees of the vertices in this graph are exactly these Fibonacci numbers.

Using Theorem 3.3, the First Zagreb Index is the sum of squared degrees:

$$M_1(G) = (F_{3k+4})^2 + (F_{3k+3})^2 + (F_{3k+2})^2.$$

By applying the well-known Fibonacci identity $F_n^2 + F_{n+1}^2 = F_{2n+1}$ (see in [11]) to the terms F_{3k+2} and F_{3k+3}, we derive the following algebraic identity:

$$M_1(G) = F_{3k+4}^2 + F_{6k+5}.$$

Remark 4.6 (Geometric Interpretation via Sum of Squares). Alternatively, using the summation identity $\sum_{i=1}^{n} F_i^2 = F_n F_{n+1}$, (see, e.g., Koshy [11]), the index $M_1(G)$ can be expressed as the difference between two partial sums:

$$M_1(G) = \sum_{i=1}^{3k+4} F_i^2 - \sum_{i=1}^{3k+1} F_i^2.$$

Applying the identity to both sums yields a compact product form:

$$M_1(G) = \begin{vmatrix} F_{3k+4} & F_{3k+1} \\ F_{3k+2} & F_{3k+5} \end{vmatrix}.$$

This result offers a geometric interpretation: the topological energy (M_1) of this Fibonacci graph corresponds precisely to the area difference between the $(3k+4)$-th and $(3k+1)$-th Golden Rectangles.

5. Conclusion and Future Work

In this paper, we have presented a unified structural framework, the $P_n(l_1, \ldots, l_n)$ graph family, which successfully generalizes the disjoint graph structures (L_q, $B_{r,s}, T_{a,b,c}, Q_{a,b,c,d}$) frequently encountered in the realization problems of number-theoretic sequences. By deriving exact general formulas for the Zagreb (M_1, M_2), Randić (R), and Harmonic (H) indices, as well as the Ω invariant, we have provided a comprehensive topological characterization of this family.

Our results go beyond mere structural analysis; they establish a tangible bridge between Graph Theory and Number Theory. We demonstrated that specific ratios of these topological indices act as "recovery operators," capable of retrieving the generating Fibonacci or Lucas numbers directly from the graph's topology. Furthermore, we showed that this topological approach preserves the asymptotic properties of the underlying sequences, such as the convergence to the Golden Ratio.

This study establishes a versatile foundation for several promising research avenues, moving beyond simple index calculations toward a more unified structural theory of sequence-based graphs. Future investigations could extend these results by exploring the behavior of other chemically significant descriptors, such as the Atom-Bond Connectivity (ABC) and Geometric-Arithmetic (GA) indices, within this generalized graph family. Moreover, the robust methodology presented here is not restricted to Fibonacci and Lucas realizations; it provides a systematic platform for investigating the topological properties of other special integer sequences, including Pell, Jacobsthal, and Padovan numbers. By bridging these diverse algebraic sequences with graph topology, this work paves the way for discovering new identities and geometric interpretations across a wide range of mathematical structures, thus offering a broader theoretical framework for future realizations.

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