

k -path graphs: experiments and conjectures about algebraic connectivity and α -index

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Abstract

This work presents conjectures about eigenvalues of matrices associated with k -path graphs, the algebraic connectivity, defined as the second smallest eigenvalue of the Laplacian matrix, and the α -index, as the largest eigenvalue of the A_α -matrix. For this purpose, a process based in [18], is presented to generate lists of k -path graphs containing all non-isomorphic 2-paths, 3-paths, and 4-paths of order n , for $6 \leq n \leq 26$, $8 \leq n \leq 19$, and $10 \leq n \leq 18$, respectively. Using these lists, exhaustive searches for extremal graphs of fixed order for the mentioned eigenvalues were performed. Based on the empirical results, conjectures are suggested about the structure of extremal k -path graphs for these eigenvalues.

Keywords: k -path graphs, Laplacian matrix, algebraic connectivity, A_α -matrix, α -index

1. Introduction

Spectral Graph Theory (SGT) studies the relationship between the structural properties of graphs and the eigenvalues of matrices associated with them.

One line of research in SGT is the determination of extremal graphs by analyzing their eigenvalues. From this perspective, we can cite several works related to some particular classes of graphs, such as paths, trees, unicyclic, bicyclic, and planar graphs, as can be seen in [22], [2], [24] and [25].

Among the Laplacian matrix's eigenvalues, the second smallest one stands out, because it has a fundamental property related to the connectivity of the graph and is called algebraic connectivity. This eigenvalue is useful in several applications, for instance, the connectivity control of mobile robot networks, in [11]; the analysis of complex directed networks with scale-free properties, in [23], and image segmentation, in [10]. Regarding A_α -matrix, it was proposed by [16] as a generalization of the signless Laplacian matrix, $Q(G)$. The signless Laplacian matrix $Q(G)$, proposed by [6], is considered by Nikiforov to be a unique matrix in several aspects, since it is the sum of the diagonal degree and adjacency matrices of a graph. Its study revealed similarities and differences between these two matrices. Currently, [16] seminal article has more than 240 citations in the Scopus database, giving rise to a line of research on linear combinations of matrices associated with graphs. Several papers about eigenvalues of A_α -matrix, in particular the largest eigenvalue, are highlighted in the bibliography.

k -Path graphs are an important subfamily of k -trees, which, in turn, are chordal graphs. k -Trees are a generalization of trees; a single vertex is a tree; adding an adjacent vertex to a single vertex of a tree with n vertices generates a new tree with $n + 1$ vertices. The definition of k -trees given in [21] is a generalization of the previous definition: a k -tree of k vertices is a complete graph of k vertices. Let T be a k -tree with n vertices, then a k -tree T' with $n + 1$ vertices is obtained from T by connecting a new vertex to each vertex of an existing clique of size k . Several problems that are NP -complete for graphs in general admit polynomial algorithms to solve them, when restricted to the class of chordal graphs, in particular k -trees (and in some cases linear ones). For this reason, chordal graphs and their subclasses are of considerable interest in the graph structure research line.

According to [4], using lists of graphs can help as a source of ideas to formulate conjectures or possible counterexamples in the study of Graph Theory. There are several web pages containing lists of graphs (e.g., the lists by Bren-

dan McKay¹, Gordon Royle², Markus Meringer³, Frank Ruskey⁴, and Ted Spence⁵. The book *Atlas of Graphs* ([20]) contains lists of drawings of various graphs, including their adjacency lists. More recently, the latest version of the graph database *House of Graphs* ([5]) provides a metadirectory containing lists of all non-isomorphic graphs up to a given order for various graph classes. The directory allows searching for graphs in the available lists.

The objective of this work is to produce lists of k -path graphs of bounded order, for $k \in \{2, 3, 4\}$ in $g6$ format. To our knowledge, there are no graph lists in $g6$ format available for k -path graphs. By using these lists, we look for information about the structure of fixed order k -path graphs that attain the largest and smallest values of some eigenvalues, algebraic connectivity, and α -index. In a previous paper ([12]), the particular case of 2-path graphs of bounded order was analyzed, and conjectures about the largest and smallest value of the algebraic connectivity were stated.

This paper is organized as follows. Section 2 presents basic concepts on Graph Theory and Spectral Graph Theory. In Section 3, information about the construction of lists of k -path graphs for fixed and limited k and n is introduced. Section 4 presents the results obtained for the experiments executed with the lists of k -path graphs. In Sections 3 and 4, the contributions of this work are given. Final remarks are presented in Section 5.

2. Basic Concepts

Let $G = (V, E)$ be an undirected graph with $|V| = n$ vertices, called the **graph order**, and $|E| = m$ edges. The neighborhood of $v \in V$ is denoted $Adj(v) = \{w \in V \mid \{v, w\} \in E\}$. The degree of v , denoted d_v , is the cardinality of its neighborhood, that is, $d_v = |Adj(v)|$. If $w \in Adj(v)$, we say that w is adjacent to v . Given $S \subset V$, the subgraph of G induced by S is denoted $G[S]$, if $G[S]$ is a complete subgraph, then S is called a **clique**. A clique of size k is denoted k -clique. A **clique** is **maximal** if it is not a proper subset (different from $\emptyset$ and the set itself) of any other clique. We denote by

¹<http://cs.anu.edu.au/~bdm/data/>

²<http://mapleta.maths.uwa.edu.au/~gordon/>

³<http://www.mathe2.unibayreuth.de/markus/reggraphs.html>

⁴<http://www.theory.cs.uvic.ca/~cos/>

⁵<http://www.maths.gla.ac.uk/~es/>

K_n , P_n , and C_n , respectively, the complete, path, and cycle graphs with n vertices. A vertex $v \in V$ is **simplicial** in G when $\text{Adj}(v)$ is a clique in G ; v is **universal** when $d_v = n - 1$. The **distance** between two vertices u and v is the length of the shortest path between them, denoted by $d(u, v)$. If there is no path between two vertices, $d(u, v) = \infty$. The **vertex connectivity** of a graph, denoted by $\kappa(G)$, is the smallest number of vertices that, when removed, make the graph disconnected. A **k -coloring** of a graph G consists of assigning to each $v \in V$ a color, from a set of k colors, in such a way that adjacent vertices receive different colors; the graph is then said to be **k -colorable**. The **chromatic number** of a graph is the smallest k such that the graph is k -colorable and denoted by $\chi(G)$. If $G = K_n$, its chromatic number is $\chi(K_n) = n$.

If $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are vertex-disjoint graphs ($V_1 \cap V_2 = \emptyset$), their graph sum is $G_1 + G_2 = (V_1 \cup V_2, E_1 \cup E_2)$. The **join** operation between two graphs, $G_1 \vee G_2$, is the graph obtained from $G_1 + G_2$ by adding new edges between each vertex of G_1 and all vertices of G_2 . Given a graph G and a positive integer d , the **d -power** of $G = (V, E)$ is the graph $G^d = (V, E')$ such that two vertices are adjacent in G^d if and only if the distance between them in G is at most d . In this work, we will frequently use the graphs $K_{k-1} \vee P_{n-k+1}$ and P_n^k , the latter called k -ribbon in [15]. For instance, the graph $K_1 \vee P_{n-1}$ is called a **fan** of order n , and the graph P_n^2 is called a **2-ribbon** of order n .

A graph $G = (V, E)$ is **chordal** if every cycle of size greater than or equal to 4 admits a chord (that is, an edge whose endpoints are non-consecutive vertices in the cycle).

A subset $S \subset V$ is a **vertex separator** for a pair of non-adjacent vertices u and v (a uv -separator) if removing S from the graph separates u and v into distinct connected components. A **minimal uv -separator** is a uv -separator that does not contain another uv -separator as a proper subset. When the vertex pair is not mentioned, S is called a **minimal vertex separator**. A **clique tree** of G is a tree T whose vertices are the maximal cliques of G such that for every pair of maximal cliques Q, Q' , the path between them in the tree T contains the intersection of these two cliques. According to [3], clique trees of chordal graphs allow represent the graph compactly and efficiently. Given a chordal graph, there exists a set of clique trees associated with this graph. It can be proved that verifying that $S \subset V$ is a minimal

vertex separator is equivalent to verifying $S = Q \cap Q'$ for some pair of maximal cliques Q, Q' , that represent vertices in a clique tree of a chordal graph. Furthermore, the set of minimal vertex separators of the chordal graph is represented in this way in any clique tree. Other definitions and results on graphs and chordal graphs can be found in [7], [3], and [9].

The **Laplacian matrix** of a graph $G = (V, E)$, where $|V| = n$, is defined as $L(G) = D(G) - A(G)$, where $D(G) = \text{diag}(d_{v_1}, \dots, d_{v_n})$ is the diagonal degree matrix of the graph's vertices and $A(G)$ is its adjacency matrix. $L(G)$ is symmetric, so it has n real eigenvalues, and it is also positive semidefinite, so all its eigenvalues are nonnegative. Furthermore, the matrix $L(G)$ is singular and therefore the smallest eigenvalue is equal to zero. The eigenvalues of $L(G)$ are denoted by $\mu_1(G) \geq \dots \geq \mu_{n-1}(G) \geq \mu_n(G) = 0$. In [8] it is proved that a graph is connected if and only if $\mu_{n-1}(G) > 0$. This eigenvalue is called **algebraic connectivity** and is denoted by $a(G)$. Fiedler also proved that the vertex connectivity is an upper bound for the algebraic connectivity of non-complete graphs.

The **signless Laplacian matrix** of a graph G , denoted by $Q(G)$, is obtained from the sum of the diagonal matrix and the adjacency matrix, $Q(G) = D(G) + A(G)$. The characteristic polynomial of this matrix Q is denoted by $p_Q(\lambda)$, and its eigenvalues (also known as Q -eigenvalues) are denoted by $q_1(G) \geq q_2(G) \geq \dots \geq q_n(G)$, with $q_1(G)$ being the largest of them, known as the **index** of $Q(G)$ or **spectral radius** of the signless Laplacian matrix.

The $A_\alpha(G)$ **matrix** is the result of a convex combination between the diagonal matrix degree and the adjacency matrix, considering any $0 \leq \alpha \leq 1$: $A_\alpha(G) = \alpha D(G) + (1 - \alpha)A(G)$. The eigenvalues of $A_\alpha(G)$ are denoted by $\lambda_1(A_\alpha) \geq \lambda_2(A_\alpha) \geq \dots \geq \lambda_n(A_\alpha)$. The spectral radius of this matrix, denoted $\rho_\alpha(G) = \lambda_1(A_\alpha)$, is called α -index. Some important relations to be highlighted are:

$$A(G) = A_0(G), \quad D(G) = A_1(G) \text{ e } Q(G) = 2A_{1/2}(G).$$

Other definitions and results on matrices and eigenvalues can be found in [1], [6] and [16].

2.1. k -path graphs

In the same article that presents the inductive definition of k -trees, [21], the following characterization of these graphs is presented. A connected

graph that has k -clique and has not $k + 2$ -clique, and for which all minimal separators induce a complete graph K_k is a k -tree.

According to [19], k -path graphs can be defined recursively as follows: let $n \geq k$ and $k \geq 2$, every complete graph with k vertices is a k -path graph. If $G = (V, E)$ is a k -path graph, and $Q \subset V$ is a k -clique containing at least one simplicial vertex, then for any vertex $v \notin V$, the augmented graph $G' = (V \cup \{v\}, E \cup \{\{v, w\} \mid w \in Q\})$ also is a k -path graph.

For k -trees, which are chordal graphs, the number of edges and the chromatic number are known ([21], [9]). Since k -path graphs verify the definition of k -tree, can be concluded that k -path graphs have $kn - \frac{k(k+1)}{2}$ edges and chromatic number $k + 1$. In this work, we consider k -paths for $k \geq 2$ and $n \geq k + 1$.

In ([14]) it is proved that maximal outerplanar graphs are 2-trees for which the clique chosen to augment the graph was not previously chosen. 2-path graphs verify this property, therefore 2-path graphs are maximal outerplanar. In the same paper, it is proved that planar 3-trees are exactly chordal and maximal planar graphs. Since 3-paths are chordal graphs, its number of edges is $3n - 6$ and they can be drawn in the plane without edge crossing, we can conclude that they are maximal planar graphs, in particular, planar. Observe that for $k \geq 4$, k -paths are non-planar graphs.

2.2. Related works

In this section, we present results from the literature on spectral parameters for k -paths and k -trees.

Let $\mathbf{T}_n^k$ be the set of all k -trees of order n . Spectral properties of k -trees are presented in [26]. Specifically, the k -path graph of fixed order with the largest eigenvalue of the signless Laplacian matrix, $q_1(G)$, is characterized, and an optimal upper bound for $q_1(G)$ in $\mathbf{T}_n^k$ is determined. Furthermore, upper bounds for $q_1(G)$ (and for related expressions such as $q_1(G) + k$, $q_1(G) - k$, $q_1(G) \cdot k$, $q_1(G)/k$) are determined for graphs G belonging to the set in $\bigcup_{k=1}^{n-1} \mathbf{T}_n^k$.

In [24] the authors defined $\mathbf{G}_n$ as the set of maximal outerplanar graphs with n vertices and no inner triangles (which are exactly the 2-path graphs). Then they proved that, the fixed order n graphs in $\mathbf{G}_n$ with $q_1(G)$ (largest eigenvalue of the unsigned Laplacian matrix) maximum and minimum are, respectively, $K_1 \vee P_{n-1}$ and P_n^2 .

In [13], the spectrum of the matrix A_α for some classes of graphs is considered, in particular, they determine the spectrum of the complete split graph, denoted $K_s \vee (n - s)K_1$, which is a particular case of k -tree.

In [25] the authors prove that the unique outerplanar graph of order n with a maximum value of α -index is $K_2 \vee P_{n-2}$. Furthermore, they prove that, if $\alpha \in [0.486, 0.5]$, the unique planar graph of order n with maximum α -index is $K_2 \vee P_{n-2}$.

In [17] the authors analyze the nullity (the multiplicity of zero as an eigenvalue of $A(G)$) of two families of k -trees, the $(k+1)$ -line graphs of k -trees and the free block-connected graphs $K_{1,k+2}$, and the simple clique k -trees, which are the k -trees whose $(k+1)$ -line graphs are trees. For each pair of integers $p \geq 2$ and $k \geq 2$, a k -tree is presented such that the nullity of its $(k+1)$ -row graph is equal to p . Furthermore, the authors establish an upper bound for the nullity of the $(k+1)$ -row graphs of k -simple clique trees with n vertices. Also, the paper demonstrates the existence of k -simple clique trees whose $(k+1)$ -row graphs have nullity between 1 and $n - (k+2) - 2\lceil \frac{n}{k+1} \rceil$.

In [12] lists of graphs are constructed, one containing maximal outerplanar graphs and the other one containing 2-path graphs, both in *g6* format and of bounded. Using these lists, conjectures about the maximal outerplanar graph and the 2-path graph, with fixed and bounded order n , that maximize and minimize algebraic connectivity are proposed.

2.3. Generating non-isomorphic k -path graphs

[18] presents a procedure that allows, given $k \geq 2$, to generate and count all non-isomorphic k -path graphs of fixed order. To this end, a coloring sequence obtained from a $(k+1)$ -coloring of the k -path graph, induced by its clique tree, is used. Regard that, according to [18], in the case of k -path graphs, the clique tree is a path.

The **core sequence** is given by $n-k$ ordered maximal cliques corresponding to the clique tree of the k -path graph. Denote the core sequence by $\mathcal{F}(G) = \langle F_1, F_2, \dots, F_{n-k} \rangle$, where $|F_i| = k+1, \forall 1 \leq i \leq n-k$. It is worth noting that for a k -path graph, there are two core sequences, because given a core sequence $\mathcal{F}(G)$, its reverse sequence, $\mathcal{F}'(G) = \langle F_{n-k}, \dots, F_1 \rangle$, is also a core sequence of G .

The intersection of two consecutive cliques in $\mathcal{F}(G)$ is a k -clique. Denote these intersections by $B_i = F_{i+1} \cap F_i$, for $i = 1, \dots, n-k$. On the other

hand, the difference of the sets corresponding to consecutive cliques, $F_{i+1} \setminus F_i$, contains a single vertex.

Let G be a k -path graph. Since G is $(k+1)$ -colorable, there exists a $k+1$ -coloring of G . The authors [18] define the **color sequence** $C = \langle c_1, c_2, \dots, c_{n-k-1} \rangle$, where c_i is the color corresponding, by the $(k+1)$ -coloring, to the vertex v_i in the sequence $\langle v_1, v_2, \dots, v_{n-k-1} \rangle$ with v_i being the only vertex in $F_{i+1} \setminus F_i$. If $n = k+1$, the color sequence is empty.

Two new concepts are introduced by [18] in order to characterize k -path graphs with fixed n by sequences of length $n - k + 1$. Given a sequence of integers of length j , $C = \langle a_1, a_2, \dots, a_j \rangle$, C is said to be **normalized** if $a_1 = 1$ and $a_i \leq 1 + \max(a_1, \dots, a_{i-1})$ for $2 \leq i \leq j$. Furthermore, if sequence C satisfies $a_i \neq a_{i+1}$ for $1 \leq i \leq j-1$ is said to be **restricted**. By using these definitions, the authors proved the two Lemmas below.

Lemma 2 (Lemma 4 [18]) Let $\mathcal{F}(G) = \langle F_1, F_2, \dots, F_{n-k} \rangle$ be a core sequence of a k -path graph with n vertices. There is a unique restricted normalized coloring sequence $C = \langle c_1, c_2, \dots, c_{n-k-1} \rangle$ of $\mathcal{F}(G)$ with at most $k+1$ colors.

Lemma 3 (Lemma 5 [18]) Let $C = \langle a_1, a_2, \dots, a_{n-k-1} \rangle$ be a restricted normalized sequence with at most $k+1$ distinct integers. C is a coloring sequence of a unique k -path graph with n vertices.

According to [18], for fixed k , the total number of k -path graphs with n vertices can be obtained as $T(n, k) = T(n-1, k-1) + M(n, k) + N(n, k)$, where $T(n-1, k-1)$ is the number of k -path graphs that has at least one universal vertex; $M(n, k)$ is the number of symmetric k -path graphs without universal vertices and $N(n, k)$ is the number of non-symmetric k -path graphs without universal vertices. As $M(n, k)$ and $N(n, k)$ can be recursively computed (equations (4) and (5) in [18]), the values of $T(n, k)$, $1 \leq k \leq 4$, are given by Table 1.

Table 1: $T(n, k)$ for $1 \leq k \leq 4$ from Table 3 [18].

	even n	odd n
$k = 1$	1	1
$k = 2$	$2^{n-6} + 2^{\frac{n-6}{2}}$	$2^{n-6} + 2^{\frac{n-7}{2}}$
$k = 3$	$\frac{3^{n-6} + 2 \cdot 3^{\frac{n-6}{2}} + 1}{4}$	$\frac{3^{n-6} + 4 \cdot 3^{\frac{n-7}{2}} + 1}{4}$
$k = 4$	$\frac{4^{n-8} + 4 \cdot 2^{n-8} + 1}{3}$	$\frac{4^{n-8} + 7 \cdot 2^{n-9} + 1}{3}$

In the next section, we will present the algorithm proposed by [18] (based on Lemmas 2 and 4) and how it will be used to produce the lists of k -path graphs with fixed and limited k and n .

3. Methodology

This section presents the 3 phases for constructing the lists of k -path graphs generated in this work. Figure 1 illustrate the construction. Given valid k and n :

phase i) Generation of color sequences representing all non-isomorphic k -path graphs with n vertices.

phase ii) For each graph, transformation of the color sequence generated in phase i) to $g6$ format.

phase iii) For fixed k , storage of the lists of k -path graphs with limited number of vertices n in *txt* files (each graph is stored in $g6$ format).

For phase i), the generation of k -path graphs proposed in [18] is used. Subsection 3.1 describes the details of the algorithm implemented for this purpose. In phase ii), *graph6* ($g6$) format was chosen to encode each graph. This format, initially presented by Brendan McKay⁶, is widely used to store graph in a compact form.

Phase iii) consists of storing in text files (*txt*) all k -path graphs, for each $k = 2, 3, 4$ and fixed and bounded n (see Figure 2).

All algorithms were implemented in a computer equipped with a 3.7 GHz AMD Ryzen 5 5600X processor and 16 GB of RAM, using the Python (v3.12.7) programming language. **NetworkX** library (v3.3) was used to generate, manipulate, and analyze the graphs. The graph images were produced with **TikZ** library, through the `tikzpicture` environment, in $\text{\LaTeX}$.

3.1. Color Sequence Generation - phase i)

In Section 2.3, theoretical results used to represent k -path graphs by restricted normalized sequences in [18] were presented. The example below illustrate the relation between k -path graphs and restricted normalized sequences.

⁶<https://users.cecs.anu.edu.au/~bdm/data/formats.txt>

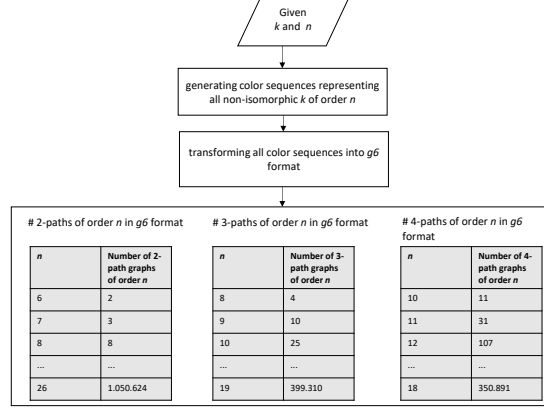


Figure 1: Construction's phases for k -path lists with $k \in \{2, 3, 4\}$ and fixed and bounded n

Given $G = P_8 \vee K_3$ of order 11 (see Figure 3). Its core sequence is given by $\mathcal{F}(G) = \langle F_1, F_2, F_3, F_4, F_5, F_6, F_7 \rangle$, with cliques $F_1 = \{u_1, u_2, u_3, v_1, v_2\}$, $F_2 = \{u_1, u_2, u_3, v_2, v_3\}$, $F_3 = \{u_1, u_2, u_3, v_3, v_4\}$, $F_4 = \{u_1, u_2, u_3, v_4, v_5\}$, $F_5 = \{u_1, u_2, u_3, v_5, v_6\}$, $F_6 = \{u_1, u_2, u_3, v_6, v_7\}$ e $F_7 = \{u_1, u_2, u_3, v_7, v_8\}$. The sequence $\langle v_3, v_4, v_5, v_6, v_7, v_8 \rangle$ is composed by vertices in the difference of sets representing consecutives 5-cliques in $\mathcal{F}(G)$, $\{v_i\} = F_{i+1} \setminus F_i$, $1 \leq i \leq n - 6$. A restricted normalized sequence of size 6 and at most 5 different integers for $G = P_8 \vee K_3$ is $C = \langle 1, 2, 1, 2, 1, 2 \rangle$.

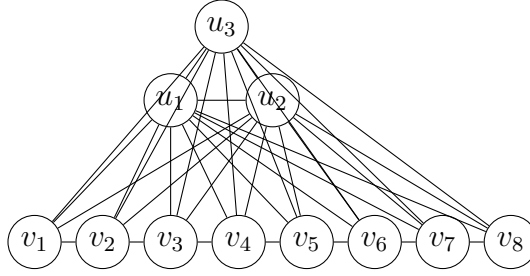


Figure 3: $P_8 \vee K_3$

The objective of Algorithm in Section 5 of [18] (see transcription in Algorithm 1 below) is to generate a restricted normalized sequences with at most $k + 1$

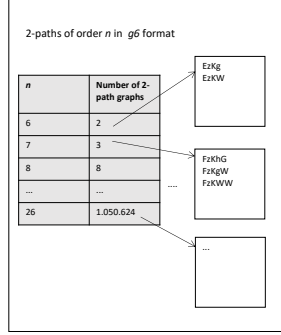


Figure 2: Details 2-path graphs lists; formats: for lists, *txt* and for graphs, *g6*

different numbers for all non-isomorphic k -path graphs, given fixed k and n , that are stored in $\mathcal{T}_{k,n}$. The algorithm considers first the smallest sequence (in lexicographic order) that satisfies the 3 conditions, $\langle 1, 2, 1, 2, 1, 2, \dots \rangle$. After that, new sequences, from the smallest one, are constructed in step 1; the definitions of restricted and normalized sequences are controlled by the variables a_i and b_i , respectively; also, the number of different integer numbers is checked. Observe that some valid sequences cannot be accepted, the reverse of each sequence must be analyzed and only the smaller one is considered (see steps a), b) and c) of the algorithm). The proof of correctness of Algorithm 1 is given in Lemmas 2 and 3 of Section 2.3.

Algorithm 1

Input: n, k .

Output: $\mathcal{T}_{k,n}$ set of color sequences of all non-isomorphic k -path graphs of order n .

1: **Step 1:**

2: Set $\langle p_1, p_2, \dots, p_{n-k-1} \rangle \leftarrow \langle 1, 2, 1, 2, \dots \rangle$

3: $\mathcal{T}_{k,n} \leftarrow \{\langle p_1, p_2, \dots, p_{n-k-1} \rangle\}$

4: **Step 2: While** exists maximu index i such that:

$$a_i = \min(\{p_{i+1}, p_{i+2}\} \setminus \{p_{i-1}\}), \quad b_i = \max(p_1, \dots, p_{i-1}) + 1, \quad a_i \leq b_i \leq 3 \mathbf{do}$$

5: **Step (a)** $\langle p_1, \dots, p_{n-k-1} \rangle \leftarrow \langle p_1, \dots, p_{i-1}, a_i, 1, 2, 1, 2, \dots \rangle$

6: **Step (b)** Compute $\langle q_1, \dots, q_{n-k-1} \rangle$ the reverse restricted normalized sequence of $\langle p_1, \dots, p_{n-k-1} \rangle$

7: **Step (c) If** $\langle p_1, \dots, p_{n-k-1} \rangle \preceq \langle q_1, \dots, q_{n-k-1} \rangle$ **then** $\mathcal{T}_{k,n} \leftarrow \mathcal{T}_{k,n} \cup \{\langle p_1, \dots, p_{n-k-1} \rangle\}$

8: **end if**

9: **end while**

10: **Return** $\mathcal{T}_{k,n}$

3.2. Transforming color sequence in g6 format - phase ii)

In this phase, the color sequences representing k -path graphs, with fixed k and n , are transformed g6 format, suitable for storage of the lists of graphs. First, the color sequence is used to construct an adjacency matrix of the graph and, from this matrix, create the compressed format g6.

The color sequence of size $n - k - 1$ represents the coloring of $n - k - 1$ vertices of the k -path graph of order n . Therefore, $k + 1$ colors of the first clique in the core sequence are conveniently added in the color sequence to obtain a $k + 1$ -coloring of the k -path graph of order n (see Section 3.1). Then, is possible to construct the adjacency matrix of the graph from the last sequence.

Finally, the g6 format is obtained by using the *networkx.Graph* function *networkx.to_graph6_bytes(G).decode('utf-8')* from the *NetworkX* library.

3.3. Storing k -path graphs in g6 format - phase iii)

In this phase, the storage of all non-isomorphic k -path graphs with fixed k and n in text files is presented.

For each value of $k = 2, 3, 4$, a text file is generated for each bounded n . A total of 41 text files were obtained: 21 for 2-path graphs ($6 \leq n \leq 26$), 12 for 3-path graphs ($8 \leq n \leq 19$), and 9 for 4-path graphs ($10 \leq n \leq 18$).

The Tables 2, 3 and 4 show the number of non-isomorphic 2-, 3-, and 4-path graphs generated for each fixed value of n .

n	# 2-paths of order n	n	# 2-paths of order n
6	2	16	1056
7	3	17	2080
8	6	18	4160
9	10	19	8256
10	20	20	16512
11	36	21	32896
12	72	22	65792
13	136	23	131328
14	272	24	262656
15	528	25	525312
		26	1050624

Table 2: Number of non-isomorphic 2-paths of order n , $6 \leq n \leq 26$.

4. Experiments and Results

This section presents experiments performed with the k -path lists generated in Section 3, as well as the analysis of the obtained results. The objective now is to determine the k -path graphs with fixed k and n in these lists that maximize (minimize) the algebraic connectivity and also maximize the α -index of the A_α -matrices for $\alpha \in \{0.1, \dots, 0.9\}$.

In order to compute extremal k -path graphs for particular eigenvalues of the Laplacian matrix and the A_α -matrix through the exhaustive exploration of the graph lists, the `np.linalg.eigvalsh()` function of NumPy library was used. In this way, the algebraic connectivity values for each of the k -path graphs of fixed order were obtained. After that, the graphs that achieves

n	# 3-paths of order n
8	4
9	10
10	25
11	70
12	196
13	574
14	1.681
15	5.002
16	14.884
17	44.530
18	133.225
19	399.310

Table 3: Number of non-isomorphic 3-paths, $8 \leq n \leq 19$.

n	# 4-paths of order n
10	11
11	31
12	107
13	379
14	1.451
15	5.611
16	22.187
17	87.979
18	350.891

Table 4: Number of non-isomorphic 4-paths, $10 \leq n \leq 18$.

its maximum and minimum values for fixed k and n were identified. For the α -index of A_α -matrix a similar process was performed. Furthermore, the second largest eigenvalue of the A_α -matrix was also analyzed

Since, for fixed k , the number of k -path graphs in $\mathcal{T}_{k,n}$ is an exponential function in n , a maximum *CPU* execution time of 1 hour was established for Algorithm 1. Therefore the largest values considered for the order of the k -path graphs with $k = 2, 3, 4$ were $n = 26, 19, 18$, respectively.

4.1. Experiments for algebraic connectivity

Tables 5 and 6 present the results obtained for the maximum and minimum algebraic connectivity, respectively, of the 2-path graphs with a fixed number of vertices, ranging from 6 to 26. The 2-path graphs, in format *g6* and their respective color sequences, that reach each of the extreme values, were identified. Note that the color sequences $\langle 1, 2, 1, 2, 1, 2, \dots \rangle$ and $\langle 1, 2, 3, 1, 2, 3, 1, 2, 3, \dots \rangle$ correspond to the graphs $K_1 \vee P_{n-1}$ and P_n^2 , for each fixed n , respectively. Therefore, in all experiments performed, the 2-path graph of fixed order n that maximizes (minimizes) the algebraic connectivity is $K_1 \vee P_{n-1}$ (P_n^2).

n	$\max_{a(G)}$	2-path G in <i>g6</i> format	C , color sequence for G
6	1.3820	EzKg	1 2 1
7	1.2679	FzKhG	1 2 1 2
8	1.1981	GzKhHC	1 2 1 2 1
9	1.1522	HxKhHC	1 2 1 2 1 2
10	1.1206	IzKhHC	1 2 1 2 1 2 1
11	1.0979	JzKhHC	1 2 1 2 1 2 1 2
12	1.0810	KzKhHC	1 2 1 2 1 2 1 2 1
13	1.0681	LzKhHC	1 2 1 2 1 2 1 2 1 2
14	1.0581	MzKhHC	1 2 1 2 1 2 1 2 1 2 1
15	1.0501	NzKhHC	1 2 1 2 1 2 1 2 1 2 1 2
16	1.0437	OzKhHC	1 2 1 2 1 2 1 2 1 2 1 2 1
17	1.0384	PzKhHC	1 2 1 2 1 2 1 2 1 2 1 2 1 2
18	1.0341	QzKhHC	1 2 1 2 1 2 1 2 1 2 1 2 1 2 1
19	1.0304	RzKhHC	1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2
20	1.0273	SzKhHC	1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1
21	1.0246	TzKhHC	1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2
22	1.0223	UzKhHC	1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1
23	1.0204	VzKhHC	1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2
24	1.0186	WzKhHC	1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2
25	1.0171	XzKhHC	1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2
26	1.0158	YzKhHC	1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2

Table 5: 2-path graph in *g6* format and its color sequence which maximizes $a(G)$ for fixed n .

n	$\min a(G)$	2-path G in $g6$ format	C , color sequence for G
6	1.1864	EzKW	1 2 3
7	0.9139	FzKWW	1 2 3 1
8	0.7186	GzKWWK	1 2 3 1 2
9	0.5778	HxKWWKB	1 2 3 1 2 3
10	0.4735	IzKWWKB?W	1 2 3 1 2 3 1
11	0.3946	JzKWWKB?W@_	1 2 3 1 2 3 1 2
12	0.3335	KzKWWKB?W@_B	1 2 3 1 2 3 1 2 3
13	0.2855	LzKWWKB?W@_B?B	1 2 3 1 2 3 1 2 3 1
14	0.2470	MzKWWKB?W@_B?B?@_	1 2 3 1 2 3 1 2 3 1 2
15	0.2158	NzKWWKB?W@_B?B?@_?W	1 2 3 1 2 3 1 2 3 1 2 3
16	0.1901	OzKWWKB?W@_B?B?@_?W?B	1 2 3 1 2 3 1 2 3 1 2 3 1
17	0.1687	PzKWWKB?W@_B?B?@_?W?B?K	1 2 3 1 2 3 1 2 3 1 2 3 1 2
18	0.1507	QzKWWKB?W@_B?B?@_?W?B?K??W	1 2 3 1 2 3 1 2 3 1 2 3 1 2 3
19	0.1354	RzKWWKB?W@_B?B?@_?W?B?K??W??W	1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1
20	0.1223	SzKWWKB?W@_B?B?@_?W?B?K??W??W??K	1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2
21	0.1110	TzKWWKB?W@_B?B?@_?W?B?K??W??W??K??B	1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3
22	0.1012	UzKWWKB?W@_B?B?@_?W?B?K??W??W??K??B??W	1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1
23	0.0927	VzKWWKB?W@_B?B?@_?W?B?K??W??W??K??B??W??@_	1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2
24	0.0852	WzKWWKB?W@_B?B?@_?W?B?K??W??W??K??B??W??@_??B	1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3
26	0.0726	YzKhGKD@G@_D?B?@_?g?H??K??g??W??S??H??W??A_??B??B??@_	1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2 3 1 2

Table 6: 2-path graph in $g6$ format and its color sequence which minimizes $a(G)$ for fixed n .

Furthermore, the corresponding graph lists were used to exhaustively determine which k -path graphs for $k = 3, 4$ have the maximum and minimum algebraic connectivity for a fixed n . In the Appendix, Tables 11, 12, 13 and 14 present the maximum and minimum algebraic connectivity value for each fixed n , ranging from 8 to 19 (for $k = 3$) and from 10 to 18 (for $k = 4$). Note that the color sequences $\langle 12 \dots 12 \dots \rangle$ and $\langle 12 \dots k+1 \dots 12 \dots k+1, \dots \rangle$ correspond to the k -path graphs $K_{k-1} \vee P_{n-k+1}$ and P_n^k . Therefore, in all experiments performed, the 3-path and 4-path graph of fixed order n that maximizes (minimizes) the algebraic connectivity are $K_1 \vee P_{n-1}$ (P_n^2).

4.2. Experiments for the eigenvalues of $A_\alpha(G)$

In this section we present results on the behavior of the largest eigenvalue of the A_α -matrices for k -path graphs, $k = 2, 3, 4$, of fixed order n . Furthermore, we investigate the second largest eigenvalue of these matrices for the same k -path graphs. The experiments will be executed for values of $\alpha \in \{0.1, 0.2, \dots, 0.9\}$.

4.2.1. The largest eigenvalue of A_α , α -index

Tables 7 and 8 present the graphs, in $g6$ format and their respective color sequences, that have the maximum α -index (for $\alpha \in \{0.1, \dots, 0.9\}$) among the 2-path graphs of fixed order n . Each row in the tables represents the

order of the graph. From Table 7 can be concluded that, for all considered values of α , the color sequence that corresponds to the graph $K_1 \vee P_{n-1}$ maximizes the α -index of the 2-path graphs of fixed order. Table 8 shows the maximum values of α -index, achieved by $K_1 \vee P_{n-1}$.

As $Q(G) = 2A_{1/2}(G)$, Tables 7 and 8 also show $2q_1(G) = 1/2$ -index. Then, the same extremal graphs were identified for the signless Laplacian index for k -path graphs of order n , with $k = 2, 3, 4$.

n	$A_{0.1}$	$A_{0.2}$	$A_{0.3}$	$A_{0.4}$	$A_{0.5}$	$A_{0.6}$	$A_{0.7}$	$A_{0.8}$	$A_{0.9}$	Color sequence
6	EzKg									1 2 1
7	FzKhG									1 2 1 2
8	GzKhHC									1 2 1 2 1
9	HzKhHC'									1 2 1 2 1 2
10	IzKhHC'GG									1 2 1 2 1 2 1
11	JzKhHC'GH?_									1 2 1 2 1 2 1 2
12	KzKhHC'GH?c@									1 2 1 2 1 2 1 2 1
13	LzKhHC'GH?c@G@									1 2 1 2 1 2 1 2 1 2
14	MzKhHC'GH?c@G@G?_									1 2 1 2 1 2 1 2 1 2 1
15	NzKhHC'GH?c@G@G?c?G									1 2 1 2 1 2 1 2 1 2 1 2
16	OzKhHC'GH?c@G@G?c?H?@									1 2 1 2 1 2 1 2 1 2 1 2 1
17	PzKhHC'GH?c@G@G?c?H?@G?C									1 2 1 2 1 2 1 2 1 2 1 2 1 2
18	QzKhHC'GH?c@G@G?c?H?@G?C_?G									1 2 1 2 1 2 1 2 1 2 1 2 1 2 1
19	RzKhHC'GH?c@G@G?c?H?@G?C_?H??G									1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2
20	SzKhHC'GH?c@G@G?c?H?@G?C_?H??H??C									1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1
21	TzKhHC'GH?c@G@G?c?H?@G?C_?H??H??C_?@									1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2
22	UzKhHC'GH?c@G@G?c?H?@G?C_?H??H??C_?@G??G									1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1
23	VzKhHC'GH?c@G@G?c?H?@G?C_?H??H??C_?@G??H???									1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2
24	WzKhHC'GH?c@G@G?c?H?@G?C_?H??H??C_?@G??H??c??@									1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1
25	XzKhHC'GH?c@G@G?c?H?@G?C_?H??H??C_?@G??H??c??@G??@									1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2
26	YzKhHC'GH?c@G@G?c?H?@G?C_?H??H??C_?@G??H??c??@G??@G???									1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1

Table 7: 2-paths with maximum α -index for fixed n . The structure of the extremal graph is the same for all $\alpha \in \{0.1, \dots, 0.9\}$.

n	0.1-index	0.2-index	0.3-index	0.4-index	0.5-index	0.6-index	0.7-index	0.8-index	0.9-index
6	3.2494	3.2835	3.3284	3.3900	3.4788	3.6127	3.8192	4.1237	4.5260
7	3.5068	3.5634	3.6401	3.7479	3.9050	4.1365	4.4670	4.9016	5.4215
8	3.7394	3.8242	3.9410	4.1070	4.3462	4.6850	5.1364	5.6897	6.3191
9	3.9555	4.0733	4.2373	4.4703	4.8003	5.2490	5.8167	6.4822	7.2177
10	4.1597	4.3145	4.5314	4.8384	5.2641	5.8227	6.5030	7.2771	8.1166
11	4.3547	4.5499	4.8247	5.2108	5.7352	6.4029	7.1929	8.0734	9.0159
12	4.5422	4.7810	5.1176	5.5868	6.2117	6.9874	7.8853	8.8706	9.9153
13	4.7237	5.0086	5.4106	5.9660	6.6922	7.5750	8.5792	9.6684	10.8149
14	4.8999	5.2334	5.7038	6.3477	7.1759	8.1649	9.2743	10.4666	11.7145
15	5.0717	5.4558	5.9973	6.7317	7.6621	8.7565	9.9703	11.2652	12.6142
16	5.2395	5.6763	6.2911	7.1175	8.1502	9.3494	10.6669	12.0639	13.5140
17	5.4038	5.8950	6.5852	7.5049	8.6400	9.9434	11.3640	12.8629	14.4138
18	5.5650	6.1123	6.8797	7.8936	9.1310	10.5381	12.0616	13.6620	15.3136
19	5.7234	6.3283	7.1745	8.2834	9.6230	11.1335	12.7594	14.4612	16.2134
20	5.8793	6.5432	7.4696	8.6742	10.1160	11.7295	13.4575	15.2605	17.1133
21	6.0328	6.7571	7.7650	9.0659	10.6097	12.3259	14.1559	16.0599	18.0132
22	6.1843	6.9700	8.0607	9.4583	11.1041	12.9227	14.8544	16.8594	18.9130
23	6.3337	7.1822	8.3566	9.8514	11.5990	13.5199	15.5530	17.6589	19.8129
24	6.4814	7.3937	8.6528	10.2450	12.0944	14.1173	16.2518	18.4584	20.7129
25	6.6274	7.6044	8.9492	10.6391	12.5902	14.7149	16.9507	19.2581	21.6128
26	6.7718	7.8146	9.2457	11.0337	13.0863	15.3128	17.6497	20.0577	22.5127

Table 8: Maximum α -index ($\alpha \in \{0.1, \dots, 0.9\}$) for 2-paths of fixed order n , $6 \leq n \leq 26$.

The same experiments were performed for 3-path and 4-path graphs. The Appendix shows Tables 15 and 16 with the results for 3-path graphs and Tables 17 and 18 for 4-path graphs. In all experiments, for all considered values of n and α , the color sequence related to the graph that achieves the maximum α -index is the sequence $\langle 12 \dots 12 \dots \rangle$, which corresponds to the graph $K_2 \vee P_{n-2}$ for 3-path and $K_3 \vee P_{n-3}$ for 4-path graphs.

4.2.2. The second largest eigenvalue of A_α , $\lambda_2(A_\alpha)$

In addition to analyzing the α -index of the k -path graphs with $k = 2, 3, 4$ and bounded order, it was considered to evaluate $\lambda_2(A_\alpha)$, the second largest eigenvalue of $A_\alpha(G)$, for $\alpha \in \{0.1, \dots, 0.9\}$.

Tables 9 and 10 present the graphs, in $g6$ format and their respective color sequences, that have the maximum $\lambda_2(A_\alpha)$ (for $\alpha \in \{0.1, \dots, 0.9\}$) among the 2-path graphs of fixed order n . Each row in the tables represents the order of the graph. From Table 9 can be concluded that, for all considered values of α , the color sequence $\langle 12 \dots 12 \dots 123 \rangle$ correspond to the graph that have maximum $\lambda_2(A_\alpha)$. Table 10 shows the maximum values of $\lambda_2(A_\alpha)$ among all 2-path graphs of fixed order n for all α .

n	$A_{0.1}$	$A_{0.2}$	$A_{0.3}$	$A_{0.4}$	$A_{0.5}$	$A_{0.6}$	$A_{0.7}$	$A_{0.8}$	$A_{0.9}$	Color sequence
6	EzKW									1 2 3
7	FzKgW									1 2 1 3
8	GzKhGK									1 2 1 2 3
9	HxKhHCB									1 2 1 2 1 3
10	IzKhHC'W									1 2 1 2 1 2 3
11	JzKhHC'GG@_									1 2 1 2 1 2 1 3
12	KzKhHC'GH?_B									1 2 1 2 1 2 1 2 3
13	LzKhHC'GH?c@?B									1 2 1 2 1 2 1 2 1 3
14	MzKhHC'GH?c@G@?@_									1 2 1 2 1 2 1 2 1 2 3
15	NzKhHC'GH?c@G@G?_?W									1 2 1 2 1 2 1 2 1 2 1 3
16	OzKhHC'GH?c@G@G?c?G?B									1 2 1 2 1 2 1 2 1 2 1 2 3
17	PzKhHC'GH?c@G@G?c?H?@??K									1 2 1 2 1 2 1 2 1 2 1 2 1 3
18	QzKhHC'GH?c@G@G?c?H?@G?C??W									1 2 1 2 1 2 1 2 1 2 1 2 1 2 3
19	RzKhHC'GH?c@G@G?c?H?@G?C_?G??W									1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 3
20	SzKhHC'GH?c@G@G?c?H?@G?C_?H??G??K									1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 3
21	TzKhHC'GH?c@G@G?c?H?@G?C_?H??H??C??B									1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 3
22	UzKhHC'GH?c@G@G?c?H?@G?C_?H??H??C_?@??W									1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 3
23	VzKhHC'GH?c@G@G?c?H?@G?C_?H??H??C_?@G??G??@_									1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 3
24	WzKhHC'GH?c@G@G?c?H?@G?C_?H??H??C_?@G??H??_??B									1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 3
25	XzKhHC'GH?c@G@G?c?H?@G?C_?H??H??C_?@G??H??c??@??B									1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 3
26	YzKhHC'GH?c@G@G?c?H?@G?C_?H??H??C_?@G??H??c??@G??@??@_									1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1 2 3

Table 9: 2-paths with maximum $\lambda_2(A_\alpha)$, of fixed order n . The structure of the extremal graph is the same for all $\alpha \in \{0.1, \dots, 0.9\}$.

n	$\lambda_2(A_{0.1})$	$\lambda_2(A_{0.2})$	$\lambda_2(A_{0.3})$	$\lambda_2(A_{0.4})$	$\lambda_2(A_{0.5})$	$\lambda_2(A_{0.6})$	$\lambda_2(A_{0.7})$	$\lambda_2(A_{0.8})$	$\lambda_2(A_{0.9})$
6	3.1996	3.2209	3.2472	3.2802	3.3229	3.3798	3.4588	3.5734	3.7456
7	3.4208	3.4541	3.4964	3.5521	3.6286	3.7388	3.9060	4.1639	4.5346
8	3.6317	3.6854	3.7567	3.8548	3.9954	4.2025	4.5046	4.9166	5.4246
9	3.8352	3.9162	4.0264	4.1815	4.4047	4.7237	5.1567	5.6974	6.3207
10	4.0319	4.1454	4.3024	4.5247	4.8404	5.2739	5.8292	6.4869	7.2186
11	4.2225	4.3728	4.5827	4.8796	5.2931	5.8399	6.5114	7.2803	8.1173
12	4.4074	4.5982	4.8660	5.2429	5.7569	6.4154	7.1990	8.0757	9.0164
13	4.5874	4.8217	5.1517	5.6124	6.2285	6.9969	7.8898	8.8723	9.9157
14	4.7629	5.0434	5.4391	5.9868	6.7056	7.5825	8.5828	9.6697	10.8152
15	4.9343	5.2635	5.7280	6.3650	7.1868	8.1709	9.2772	10.4677	11.7147
16	5.1022	5.4822	6.0181	6.7462	7.6711	8.7614	9.9726	11.2660	12.6144
17	5.2667	5.6996	6.3091	7.1299	8.1578	9.3535	10.6689	12.0647	13.5141
18	5.4284	5.9157	6.6010	7.5155	8.6464	9.9468	11.3657	12.8635	14.4139
19	5.5873	6.1309	6.8936	7.9028	9.1365	10.5411	12.0630	13.6625	15.3137
20	5.7437	6.3450	7.1869	8.2915	9.6279	11.1361	12.7606	14.4617	16.2135
21	5.8979	6.5584	7.4807	8.6814	10.1202	11.7318	13.4586	15.2609	17.1134
22	6.0500	6.7709	7.7750	9.0723	10.6135	12.3279	14.1568	16.0603	18.0132
23	6.2001	6.9827	8.0697	9.4640	11.1074	12.9245	14.8552	16.8597	18.9131
24	6.3484	7.1938	8.3648	9.8565	11.6020	13.5215	15.5538	17.6592	19.8130
25	6.4951	7.4043	8.6602	10.2496	12.0970	14.1187	16.2525	18.4587	20.7129
26	6.6401	7.6143	8.9559	10.6433	12.5926	14.7162	16.9514	19.2583	21.6128

Table 10: Maximum $\lambda_2(A_\alpha)$ ($\alpha \in \{0.1, \dots, 0.9\}$) for 2-paths with fixer order n , $6 \leq n \leq 26$.

The same experiments were performed for 3-path and 4-path graphs. The

Appendix shows Tables 19 and 20 with the results for 3-paths and Tables 21 and 22 for 4-paths. In all experiments, for all considered values of n and α , the color sequence related to the graph that achieves the maximum $\lambda_2(A_\alpha)$ for 3-path and 4-path graphs has color sequence $\langle 1\ 2\ \dots\ 1\ 2\ \dots\ 1\ 2\ 3 \rangle$. Tables 20 and 22 show the maximum values of $\lambda_2(A_\alpha)$ among all 3-path and 4-paths, respectively, of fixed order n for all α considered.

4.3. Conjectures

By observing the structural patterns of k -path graphs, as well as the results for the maximum and minimum algebraic connectivities, is possible to formulate a conjecture about the k -path graphs with $k \geq 2$ and fixed n that maximize and minimize the algebraic connectivity.

Conjecture 4.1. *Given fixed $n \geq k + 1$ and $k \geq 2$, the unique k -path graph that maximizes the algebraic connectivity is $K_{k-1} \vee P_{n-k+1}$. Moreover, in the same conditions, the unique k -path graph that minimizes the algebraic connectivity is P_n^k .*

On the other hand, for A_α -matrix, the experiments executed for k -path graphs, $k = 2, 3, 4$, bounded order n and $\alpha \in \{0.1, \dots, 0.9\}$ allow us to formulate the following conjecture involving the maximum α -index and the maximum $\lambda_2(A_\alpha)$ for k -path graphs.

First, we introduce the definition of a particular k -path graph of order n . Graph $K_{k-1} \vee P_{n-k+1}$ is called **k -generalized-fan** of order n and its restricted normalized sequence is given by $\langle 1, 2, 1, 2, \dots, 1, 2 \rangle$. The **k -weak-generalized-fan** of order n is the unique k -path G , unless isomorphism, such that there exists a vertex v for which $G - v = K_{k-1} \vee P_{n-1-k+1}$. The restricted normalized sequence for the k -weak-generalized-fan graph of order n is the sequence of size $n - k + 1$ given by $\langle 1, 2, 1, 2, \dots, 1, 2, 3 \rangle$. Figures 3 and 4 show the 2-generalized-fan and 2-weak-generalized-fan graphs of order 7, respectively.

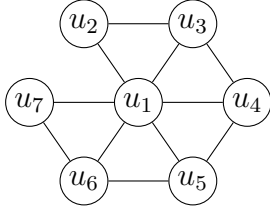


Figure 3: 2-generalized fan of order 7

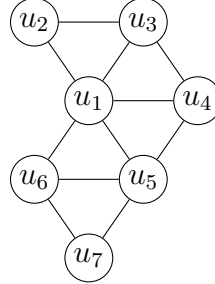


Figure 4: 2-weak-generalized-fan of order 7

Conjecture 4.2. *Given fixed $n \geq k + 1$ and $k \geq 2$ the unique k -path graph that maximizes α -index for $\alpha \in [0, 1]$ is $K_{k-1} \vee P_{n-k+1}$. Moreover, in the same conditions, the unique k -path graph that maximizes $\lambda_2(A_\alpha)$ is the k -weak-generalized-fan.*

5. Conclusions

In this work, we present lists of k -path graphs for $k \in \{2, 3, 4\}$ and bounded order in $g6$ format. The following ranges for the number of vertices were considered: $6 \leq n \leq 26$ for 2-paths, $8 \leq n \leq 19$ for 3-paths, and $8 \leq n \leq 18$ for 4-paths. These lists were used, extensively, to obtain information about the behavior of the eigenvalues of the Laplacian and the A_α -matrices. As a result of this work, given fixed $n \geq k + 1$ and a bounded n , it was possible to identify the structure of the k -path graph that maximizes or minimizes the algebraic connectivity, and maximizes the α -index, and the second largest eigenvalue of $A_\alpha(G)$ ($\lambda_2(A_\alpha)$), for $\alpha \in \{0.1, \dots, 0.9\}$. Finally, two conjectures were proposed regarding the mentioned eigenvalues.

It is worth mentioning that all the experimental results obtained in this work for 2-path and 3-path graphs are consistent with the theorems and conjectures set in [24] and [25] for outerplanar and planar graphs. However, 4-path graphs are non-planar, and to our knowledge, do not exist other works in the literature about extremal graphs for the algebraic connectivity or α -index of k -path graphs with $k \geq 4$.

The obtained results allow identifying research problems to be addressed. For instance, to find a formal proof of the conjectures presented here, as well as the use of the lists of k -path graphs to determine new conjectures in Graph Theory and Spectral Graph Theory.

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7. Appendix

7.1. Maximum and minimum algebraic connectivity of 3-paths and 4-paths of fixed order n

n	$\max a(G)$	3-path G in $g6$ format	C , color sequence for G
8	2.2679	$G \sim [xhc$	1 2 1 2
9	2.1981	$H \sim [xhcp$	1 2 1 2 1
10	2.1522	$I \sim [xhcpKG$	1 2 1 2 1 2
11	2.1206	$J \sim [xhcpKH_$	1 2 1 2 1 2 1
12	2.0979	$K \sim [xhcpKH_e@$	1 2 1 2 1 2 1 2
13	2.0810	$L \sim [xhcpKH_e@K@$	1 2 1 2 1 2 1 2 1
14	2.0681	$M \sim [xhcpKH_e@K@K?e?G$	1 2 1 2 1 2 1 2 1 2
15	2.0581	$N \sim [xhcpKH_e@K@K?e?H_@$	1 2 1 2 1 2 1 2 1 2 1
16	2.0501	$O \sim [xhcpKH_e@K@K?e?H_@K?C$	1 2 1 2 1 2 1 2 1 2 1 2
17	2.0437	$P \sim [xhcpKH_e@K@K?e?H_@K?Co?G$	1 2 1 2 1 2 1 2 1 2 1 2 1
18	2.0384	$Q \sim [xhcpKH_e@K@K?e?H_@K?Co?G$	1 2 1 2 1 2 1 2 1 2 1 2 1 2
19	2.0341	$R \sim [xhcpKH_e@K@K?e?H_@K?Co?H_?G$	1 2 1 2 1 2 1 2 1 2 1 2 1 2 1

Table 11: 3-path graph, in $g6$ format and its color sequence, which maximizes $a(G)$ for fixed n .

n	$\min a(G)$	3-path G in $g6$ format	C , color sequence for G
8	1.7926	$G \sim [ww[$	1 2 3 4
9	1.4854	$H \sim [ww[F$	1 2 3 4 1
10	1.2430	$I \sim [ww[F?w$	1 2 3 4 1 2
11	1.0502	$J \sim [ww[F?wB_$	1 2 3 4 1 2 3
12	0.8968	$K \sim [ww[F?wB_F$	1 2 3 4 1 2 3 4
13	0.7733	$L \sim [ww[F?wB_F?F$	1 2 3 4 1 2 3 4 1
14	0.6729	$M \sim [ww[F?wB_F?F?B_$	1 2 3 4 1 2 3 4 1 2
15	0.5903	$N \sim [ww[F?wB_F?F?B_?w$	1 2 3 4 1 2 3 4 1 2 3
16	0.5217	$O \sim [ww[F?wB_F?F?B_?w?F$	1 2 3 4 1 2 3 4 1 2 3 4
17	0.4642	$P \sim [ww[F?wB_F?F?B_?w?F??[$	1 2 3 4 1 2 3 4 1 2 3 4 1
18	0.4156	$Q \sim [ww[F?wB_F?F?B_?w?F??[??w$	1 2 3 4 1 2 3 4 1 2 3 4 1 2
19	0.3742	$R \sim [ww[F?wB_F?F?B_?w?F??[??w??w$	1 2 3 4 1 2 3 4 1 2 3 4 1 2 3

Table 12: 3-path graph, in $g6$ format and its color sequence, which minimizes $a(G)$ for fixed n .

n	$\max a(G)$	4-path G in $g6$ format	C , color sequence for G
10	3.1981	I~ xxsxMG	1 2 1 2 1
11	3.1522	J~ xxsxMHo_	1 2 1 2 1 2
12	3.1206	K~ xxsxMHof@	1 2 1 2 1 2 1
13	3.0979	L~ xxsxMHof@M@	1 2 1 2 1 2 1 2
14	3.0810	M~ xxsxMHof@M@M?_	1 2 1 2 1 2 1 2 1
15	3.0681	N~ xxsxMHof@M@M?f?G	1 2 1 2 1 2 1 2 1 2
16	3.0581	O~ xxsxMHof@M@M?f?Ho@	1 2 1 2 1 2 1 2 1 2 1
17	3.0501	P~ xxsxMHof@M@M?f?Ho@M?C	1 2 1 2 1 2 1 2 1 2 1 2
18	3.0437	Q~ xxsxMHof@M@M?f?Ho@M?Cw?G	1 2 1 2 1 2 1 2 1 2 1 2 1

Table 13: 4-path graph, in $g6$ format and its color sequence, which maximizes $a(G)$ for fixed n .

n	$\min a(G)$	4-path G in $g6$ format	C , color sequence for G
10	2.4015	I~ xw{N@w	1 2 3 4 5
11	2.0737	J~ xw{N@wF_	1 2 3 4 5 1
12	1.8007	K~ xw{N@wF_N	1 2 3 4 5 1 2
13	1.5722	L~ xw{N@wF_N?N	1 2 3 4 5 1 2 3
14	1.3804	M~ xw{N@wF_N?N?F_	1 2 3 4 5 1 2 3 4
15	1.2196	N~ xw{N@wF_N?N?F_@w	1 2 3 4 5 1 2 3 4 5
16	1.0839	O~ xw{N@wF_N?N?F_@w?N	1 2 3 4 5 1 2 3 4 5 1
17	0.9687	P~ xw{N@wF_N?N?F_@w?N??{	1 2 3 4 5 1 2 3 4 5 1 2
18	0.8703	Q~ xw{N@wF_N?N?F_@w?N??{?@w	1 2 3 4 5 1 2 3 4 5 1 2 3

Table 14: 4-path graph, in $g6$ format and its color sequence, which minimizes $a(G)$ for fixed n .

7.2. Largest α -index for $\alpha \in \{0.1, \dots, 0.9\}$

n	$A_{0.1}$	$A_{0.2}$	$A_{0.3}$	$A_{0.4}$	$A_{0.5}$	$A_{0.6}$	$A_{0.7}$	$A_{0.8}$	$A_{0.9}$	Color sequence
8	G~[xhc									1 2 1 2
9	H~[xhcp									1 2 1 2 1
10	I~[xhcpKG									1 2 1 2 1 2
11	J~[xhcpKH_									1 2 1 2 1 2 1
12	K~[xhcpKH_e@									1 2 1 2 1 2 1 2
13	L~[xhcpKH_e@K@									1 2 1 2 1 2 1 2 1
14	M~[xhcpKH_e@K@K?_									1 2 1 2 1 2 1 2 1 2
15	N~[xhcpKH_e@K@K?e?G									1 2 1 2 1 2 1 2 1 2 1
16	O~[xhcpKH_e@K@K?e?H_@									1 2 1 2 1 2 1 2 1 2 1 2
17	P~[xhcpKH_e@K@K?e?H_@K?C									1 2 1 2 1 2 1 2 1 2 1 2 1
18	Q~[xhcpKH_e@K@K?e?H_@K?Co?G									1 2 1 2 1 2 1 2 1 2 1 2 1 2
19	R~[xhcpKH_e@K@K?e?H_@K?Co?H_?G									1 2 1 2 1 2 1 2 1 2 1 2 1 2 1

Table 15: 3-paths with maximum α -index for fixed n . The structure of the extremal graph is the same for all $\alpha \in \{0.1, \dots, 0.9\}$.

n	0.1-index	0.2-index	0.3-index	0.4-index	0.5-index	0.6-index	0.7-index	0.8-index	0.9-index
8	4.8793	4.9308	4.9976	5.0867	5.2094	5.3832	5.6322	5.9813	6.4412
9	5.1982	5.2751	5.3756	5.5101	5.6946	5.9504	6.3017	6.7646	7.3371
10	5.4946	5.6007	5.7400	5.9267	6.1803	6.5245	6.9799	7.5536	8.2344
11	5.7738	5.9124	6.0948	6.3388	6.6673	7.1037	7.6637	8.3458	9.1326
12	6.0392	6.2130	6.4422	6.7481	7.1556	7.6868	8.3512	9.1400	10.0312
13	6.2932	6.5046	6.7839	7.1554	7.6453	8.2729	9.0413	9.9354	10.9302
14	6.5377	6.7888	7.1210	7.5612	8.1361	8.8612	9.7333	10.7318	11.8293
15	6.7739	7.0667	7.4542	7.9659	8.6279	9.4512	10.4266	11.5289	12.7287
16	7.0030	7.3391	7.7843	8.3698	9.1205	10.0427	11.1210	12.3265	13.6281
17	7.2257	7.6068	8.1116	8.7731	9.6139	10.6353	11.8162	13.1244	14.5276
18	7.4428	7.8703	8.4366	9.1759	10.1080	11.2288	12.5121	13.9226	15.4272
19	7.6549	8.1300	8.7597	9.5782	10.6026	11.8231	13.2086	14.7211	16.3269

Table 16: Maximum α -index ($\alpha \in \{0.1, \dots, 0.9\}$) for 3-paths of fixed order, $8 \leq n \leq 19$.

n	$A_{0.1}$	$A_{0.2}$	$A_{0.3}$	$A_{0.4}$	$A_{0.5}$	$A_{0.6}$	$A_{0.7}$	$A_{0.8}$	$A_{0.9}$	Color sequence
10	$I^- xxsxMG$									1 2 1 2 1
11	$J^- xxsxMHo_$									1 2 1 2 1 2
12	$K^- xxsxMHof@$									1 2 1 2 1 2 1
13	$L^- xxsxMHof@M@$									1 2 1 2 1 2 1 2
14	$M^- xxsxMHof@M@M?_$									1 2 1 2 1 2 1 2 1
15	$N^- xxsxMHof@M@M?f?G$									1 2 1 2 1 2 1 2 1 2
16	$O^- xxsxMHof@M@M?f?Ho@$									1 2 1 2 1 2 1 2 1 2 1
17	$P^- xxsxMHof@M@M?f?Ho@M?C$									1 2 1 2 1 2 1 2 1 2 1 2
18	$Q^- xxsxMHof@M@M?f?Ho@M?Cw?G$									1 2 1 2 1 2 1 2 1 2 1 2 1

Table 17: 4-paths with maximum α -index for fixed n . The structure of the extremal graph is the same for all $\alpha \in \{0.1, \dots, 0.9\}$.

n	0.1-index	0.2-index	0.3-index	0.4-index	0.5-index	0.6-index	0.7-index	0.8-index	0.9-index
10	6.5111	6.5784	6.6646	6.7775	6.9295	7.1386	7.4295	7.8290	8.3539
11	6.8634	6.9567	7.0764	7.2333	7.4431	7.7273	8.1113	8.6167	9.2504
12	7.1952	7.3174	7.4744	7.6799	7.9530	8.3173	8.7970	9.4076	10.1478
13	7.5104	7.6639	7.8615	8.1198	8.4605	8.9085	9.4855	10.2008	11.0460
14	7.8117	7.9988	8.2399	8.5543	8.9663	9.5008	10.1762	10.9953	11.9445
15	8.1012	8.3238	8.6109	8.9847	9.4709	10.0941	10.8684	11.7910	12.8434
16	8.3805	8.6405	8.9759	9.4115	9.9746	10.6881	11.5618	12.5873	13.7425
17	8.6510	8.9498	9.3356	9.8356	10.4776	11.2828	12.2562	13.3843	14.6417
18	8.9135	9.2527	9.6908	10.2572	10.9802	11.8781	12.9513	14.1817	15.5410

Table 18: Maximum α -index ($\alpha \in \{0.1, \dots, 0.9\}$) for 4-paths of fixed order, $8 \leq n \leq 18$.

7.3. Largest $\lambda_2(A_\alpha)$ for $\alpha \in \{0.1, \dots, 0.9\}$

n	$A_{0.1}$	$A_{0.2}$	$A_{0.3}$	$A_{0.4}$	$A_{0.5}$	$A_{0.6}$	$A_{0.7}$	$A_{0.8}$	$A_{0.9}$	Color sequence
8	$G^- [xgk]$									1 2 1 3
9	$H^- [xhcR]$									1 2 1 2 3
10	$I^- [xhcpCW]$									1 2 1 2 1 3
11	$J^- [xhcpKG'_-]$									1 2 1 2 1 2 3
12	$K^- [xhcpKH_aB]$									1 2 1 2 1 2 1 3
13	$L^- [xhcpKH_e@CB]$									1 2 1 2 1 2 1 2 3
14	$M^- [xhcpKH_e@K@K?a?W]$									1 2 1 2 1 2 1 2 1 3
15	$N^- [xhcpKH_e@K@K?e?G_B]$									1 2 1 2 1 2 1 2 1 2 3
16	$O^- [xhcpKH_e@K@K?e?H_@C?K]$									1 2 1 2 1 2 1 2 1 2 1 2 3
17	$P^- [xhcpKH_e@K@K?e?H_@K?CO?W]$									1 2 1 2 1 2 1 2 1 2 1 2 1 3
18	$Q^- [xhcpKH_e@K@K?e?H_@K?Co?G_?W]$									1 2 1 2 1 2 1 2 1 2 1 2 1 2 3
19	$R^- [xhcpKH_e@K@K?e?H_@K?Co?G_?W]$									1 2 1 2 1 2 1 2 1 2 1 2 1 2 3

Table 19: 3-paths with maximum $\lambda_2(A_\alpha)$ for fixed n . The structure of the extremal graph is the same for all $\alpha \in \{0.1, \dots, 0.9\}$.

n	$\lambda_2(A_{0.1})$	$\lambda_2(A_{0.2})$	$\lambda_2(A_{0.3})$	$\lambda_2(A_{0.4})$	$\lambda_2(A_{0.5})$	$\lambda_2(A_{0.6})$	$\lambda_2(A_{0.7})$	$\lambda_2(A_{0.8})$	$\lambda_2(A_{0.9})$
8	4.8208	4.8612	4.9132	4.9825	5.0791	5.2216	5.4452	5.8063	6.3397
9	5.1250	5.1877	5.2694	5.3796	5.5337	5.7579	6.0923	6.5823	7.2354
10	5.4123	5.5020	5.6198	5.7791	6.0006	6.3148	6.7603	7.3691	8.1331
11	5.6857	5.8061	5.9650	6.1798	6.4753	6.8838	7.4389	8.1607	9.0316
12	5.9474	6.1016	6.3058	6.5810	6.9554	7.4606	8.1237	8.9549	9.9306
13	6.1991	6.3897	6.6426	6.9824	7.4392	8.0424	8.8123	9.7506	10.8298
14	6.4420	6.6714	6.9761	7.3839	7.9258	8.6279	9.5034	10.5473	11.7292
15	6.6773	6.9475	7.3066	7.7853	8.4145	9.2161	10.1963	11.3446	12.6288
16	6.9058	7.2186	7.6346	8.1867	8.9049	9.8062	10.8904	12.1425	13.5284
17	7.1283	7.4854	7.9604	8.5880	9.3965	10.3978	11.5856	12.9407	14.4281
18	7.3454	7.7483	8.2842	8.9891	9.8892	10.9907	12.2815	13.7393	15.3278
19	7.5575	8.0076	8.6062	9.3902	10.3828	11.5844	12.9780	14.5380	16.2276

Table 20: Maximum $\lambda_2(A_\alpha)$ ($\alpha \in \{0.1, \dots, 0.9\}$) for 3-paths of fixed order, $8 \leq n \leq 19$.

n	$A_{0.1}$	$A_{0.2}$	$A_{0.3}$	$A_{0.4}$	$A_{0.5}$	$A_{0.6}$	$A_{0.7}$	$A_{0.8}$	$A_{0.9}$	Color sequence
10	$I^- xxsxEW$									1 2 1 2 3
11	$J^- xxsxMGp_-$									1 2 1 2 1 3
12	$K^- xxsxMHobB$									1 2 1 2 1 2 3
13	$L^- xxsxMHof@EB$									1 2 1 2 1 2 1 3
14	$M^- xxsxMHof@M@E@_-$									1 2 1 2 1 2 1 2 3
15	$N^- xxsxMHof@M@M?b?W$									1 2 1 2 1 2 1 2 1 3
16	$O^- xxsxMHof@M@M?f?GoB$									1 2 1 2 1 2 1 2 1 2 3
17	$P^- xxsxMHof@M@M?f?Ho@E?K$									1 2 1 2 1 2 1 2 1 2 1 3
18	$Q^- xxsxMHof@M@M?f?Ho@M?CW?W$									1 2 1 2 1 2 1 2 1 2 1 2 3

Table 21: 4-path with maximum $\lambda_2(A_\alpha)$ for fixed n . The structure of the extremal graph is the same for all $\alpha \in \{0.1, \dots, 0.9\}$.

n	$\lambda_2(A_{0.1})$	$\lambda_2(A_{0.2})$	$\lambda_2(A_{0.3})$	$\lambda_2(A_{0.4})$	$\lambda_2(A_{0.5})$	$\lambda_2(A_{0.6})$	$\lambda_2(A_{0.7})$	$\lambda_2(A_{0.8})$	$\lambda_2(A_{0.9})$
10	6.4563	6.5149	6.5898	6.6885	6.8228	7.0124	7.2880	7.6928	8.2652
11	6.8015	6.8847	6.9915	7.1325	7.3234	7.5881	7.9599	8.4762	9.1612
12	7.1286	7.2396	7.3826	7.5711	7.8245	8.1699	8.6399	9.2651	10.0587
13	7.4406	7.5821	7.7648	8.0051	8.3258	8.7556	9.3250	10.0572	10.9569
14	7.7397	7.9142	8.1396	8.4355	8.8272	9.3442	10.0135	10.8512	11.8555
15	8.0278	8.2372	8.5080	8.8626	9.3285	9.9348	10.7042	11.6465	12.7545
16	8.3061	8.5523	8.8710	9.2871	9.8297	10.5269	11.3967	12.4428	13.6536
17	8.5759	8.8606	9.2292	9.7092	10.3309	11.1202	12.0904	13.2397	14.5529
18	8.8381	9.1627	9.5832	10.1294	10.8319	11.7144	12.7851	14.0371	15.4524

Table 22: Maximum $\lambda_2(A_\alpha)$ ($\alpha \in \{0.1, \dots, 0.9\}$) for 4-paths of fixed order, $10 \leq n \leq 18$.