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Extreme Topologies on Bipolygonal Graphs and Dinamic Trees

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Abstract. We show how properties of the sequence $\beta_{i,j}$, which represents the product between two Fibonacci's numbers $F_i \cdot F_j$, can be used for the computation of the Merrifield-Simmons index on bipolygonal graphs and trees.
We show that the extreme values of the Merrifield-Simmons index on bipolygonal graphs are found in two consecutive columns of the table $\beta_{i,j}$ k=i+j=1,...,n. The minimum value in $\beta_{3,k-3}$ and the maximum value in $\beta_{4,k-4}$. On the other hand we show that $i(T_n \cup \{\{v_p, v\}\})$ is minimum when v is a new leaf node, and its father v_p was also a leaf node in T_n.
Our methods does not require the explicit computation of the number of independent sets of the involved graphs. Instead, it is based on applying the edge and vertex division rules to decompose the initial graph.
Keywords: Counting independent sets, Merrifield-Simmons index, Extremal topologies, Bipolygonal graphs, Trees, Structural pattern recognition.

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1 Introduction

The recognition of extremal topologies on graphs has been a significant study on the structural pattern recognition area [17]. Especially in graph theory, several works deal with the characterization of extremal graphs concerning Hosoya and Merrifield-Simmons indices containing pentagonal and hexagonal cycles.

Merrifield and Simmons showed the correlation between the number of independent sets of G, denoted by i(G), and the boiling points of the molecular graph represented by G in [13]. This fact is one of the main reasons why the number of independent sets of a graph G, in mathematical chemistry, is called the Merrifield-Simmons index (M-S) of G. However, in graph theory, i(G) is called the Fibonacci number of G. The Fibonacci numbers and their properties have been useful in analyzing structural compounds in mathematical chemistry.

The Merrifield-Simmons index is a significant topological index of the structural chemistry of the molecular graph G [16,17]. A topological index is a map from the set of chemical compounds represented by molecular graphs to the set of real numbers. Many topological indices are closely correlated with some physicochemical characteristics of the underlying compounds. The Merrield-Simmons index is a topological index whose mathematical properties appeared in some detail in [10]. The M-S and Hosoya indices are some of the most popular topological indices in chemistry.

Hexagonal array graphs have been widely investigated. They represent a relevant area of interest in mathematical chemistry because they have been used to study the intrinsic properties of molecular graphs. Phenylene is any divalent aromatic radical obtained from a benzene molecule by removing two hydrogen atoms. Many of the polymers in which the basic building block is phenylene are called polyphenylene.

A special class of graphs represented by two polygons joined by an edge is the basic graphs representing Polyphenylenes compounds. Unbranched polyphenylenes appear in the context of low-dimensional organic conductors, while their dendrimer-like counterparts play an important role in synthesizing large graphene molecules [8].

The recognition of extremal topologies on graphs has been a significant study on the pattern structural recognition area [17]. Especially, in graph theory, several works deal with the characterization of extremal graphs with respect to Hosoya and Merrifield-Simmons indices for different topology graphs, such as trees, unicyclic graphs, and certain structures containing pentagonal and hexagonal cycles [5,7,16,17,23,24]. For example, Ren et al. [14] determined the minimal Merrifield-Simmons index of double hexagonal chains. In [15], Gutman et al. characterized the tree with the maximal Merrifield-Simmons index among the trees with a given diameter. In [19], a survey about extremal graphs for Hosoya and Merrifield-Simmons indices considered different graph topologies.

In the case of trees, it is known that the topology with a minimum number of independent sets corresponds to the path $i(P_n) = F_{n+2}$. Meanwhile, the topology with the maximum value for the number of independent sets correspond to the start: $i(S_n) = 2^{n-1} +1$ [25]. In [22], the largest number of maximal independent sets that any tree T_n of order n can have is determined. This work also shows a linear time algorithm for the computation of the number of maximal independent sets for any input tree.

Two of the works related to our analysis to determine extremal values for the M-S index on trees are the works of Li et al. [10] and Lv et al. [21]. In [10], the maximum value for $i(T(n, k))$, which corresponds to the tree of n vertices and diameter k, is determined. Meanwhile, in [21] Lv et al. shows how to determine the topology for the tree of n vertices with maximum degree k and which, at the same time, corresponds to the maximum value for the M-S index. In comparison to their methods of fixing the tree parameters, in our analysis we consider any input tree T_n of order n. As a matter of fact, the initial topology of T_n will change, since a new leaf node v will be inserted to T_n. Therefore, a dynamic topology for the input tree should be considered. We determine the topology that must have $T_n \cup \{\{v_p, v\}\})$ with $vp \in V(T_n), v \notin V(T_n)$ that corresponds with the extremal values (maximum and minimum) of the M-S index on any tree $T_n \cup \{\{v_p, v\}\})$.

On the other hand, several works analyze product sequences among Fibonacci numbers. For example, Adegoke [1] derived infinite product identities involving Fibonacci and Lucas numbers. In [4], it is shown that the generating function of the Fibonacci sequence produces values that constitute all rational numbers; in [9] developed a generalization about two proven Fibonacci-Lucas identities. In [18], the main result is the obtention of identity by the m-th power of Fibonacci numbers in which the subscripts of the involved Fibonacci numbers are arbitrarily spaced as their dual identities.

In [3], several results proved the convergence of the minimum and maximum higher-order recurrences for maximum and minimum Fibonacci values. At the same time, in [2], some properties of the m-sequences system were defined by recurrence relation using a matricial product.

In this paper, we show how properties of the product between two Fibonacci's numbers and the application of the edge division rule can be used for the computation of extremal values of the Merrifield-Simmons index on a bipolygonal graph and dynamic trees.

In the following section, we introduce some needed notations for this paper. In section the Fibonaccis products is proposed, while in sections four and five show the analysis for obtaining extremal values for the Merrifield-Simmons index on bipolygonal graphs and dynamic trees. The last section presents the conclusions.

2 Preliminary concepts

Let G=(V, E) be an undirected graph with vertices set V and set of edges E. G is assumed to be a simple graph with no loops or parallel edges. The neighborhood of $x \in V$ is the set $N(x) = \{y \in V : xy \in E\}$, and its closed neighborhood is $N(x) \cup \{x\}$ which is denoted by $N[x]$. The degree of a vertex x in a graph G, denoted by $\delta_G(x)$, is $|N(x)|$. The degree of the graph G is $\Delta(G) = \max\{\delta_G(x): x \in V\}$.

A path between two vertex v and w, denoted as P_{vw} or simply as P_n, is a sequence of the edges: $v_0v_1, v_1v_2, \ldots, v_{n-1}v_n$ such that $v=v_0$, $v_n=w$, and $v_kv_{k+1} \in E$ for $0 \leq k< n$; the length of the path is n. A simple path is a path where $v_0, v_1,\ldots, v_{n-1}, v_n$ are all distinct. A cycle is a non-empty path such that the first and last vertices are identical, and a simple cycle is a cycle in which no vertex is repeated except that the first and last vertices are identical.

A subset $S \subseteq V$ is called independent if, for every $u,v \in S$ implies that $uv \notin E$. The corresponding counting problem on independent sets, denoted by $i(G)$, consists of counting the number of independent sets of a graph G. To compute $i(G)$ is a #P-complete problem for graphs G where $\Delta(G) \geq 3$. Computation of $i(G)$ remains #P-complete even if it is restricted to 3-regular graphs [6].

Let G=(V, E) be a molecular graph. Denote by n(G, k) the number of ways in which k mutually independent vertices can be selected in G. By definition, n(G, 0) = 1 for all graphs, and n(G, 1) = |V(G)|. Furthermore, $i(G) = \sum_{k\geq 0} n(G,k)$ is the Merrifield-Simmons index of G, that is, exactly the number of independent sets of G.

A polygon (also called a polygonal graph) is a simple cycle graph. Therefore, a cycle graph C_n of length n represents a polygon of n sides, and it forms a n-gon. The way that two k-gons are joined, via a common vertex or via a common edge defines different classes of polygonal chemical compounds. Two polygons that have an edge in common are called adjacent.

A polygonal chain is a 2-connected simple graph G obtained by identifying a finite number of congruent regular polygons (called basic polygons) one by one such that each vertex of G has degree 2 or 3, and each basic polygon, except the first one and the last one, is adjacent to exactly two basic polygons. A polygonal array is a graph $P_{k,t}$ obtained by identifying a finite number of t congruent polygons. When each polygon in $P_{k,t}$ has the same number of k sides, then $P_{k,t}$ becomes in a chain of t k-gons.

In this work, we analyze the case of $P_{k,2}$, this is, a bipolygonal graph, where k will be the total number of vertices involved in both polygons. This class of bipolygonal graphs are the polygonal extremes of a chain of phenylenes or bypiridines chemical compounds.

An acyclic graph is a graph that does not contain cycles. The connected acyclic graphs are called trees, and a connected graph is a graph where for any pair of vertices, there is a path connecting them. It is not difficult to infer that in a tree, there is a unique path connecting any two pairs of its vertices. We denote by P_n, T_n, S_n, and K_n to the path, tree, start graph, and complete graph, respectively, all containing n vertices.

Some reduction rules have been useful in counting combinatorial objects on graphs. Particularly, the following rules are commonly used:

1. Vertex reduction rule: let $v \in V(G)$,

$$i(G) = i(G - v) + i(G - (N[v])) . \tag{1}$$

2. Edge division rule : let $e= \{x, y\} \in E(G)$,

$$i(G) = i(G - e) - i(G - (N[x] \cup N[y])) . \tag{2}$$

3 The product between Fibonacci Numbers with complementary indexes

Let us denote the n-th Fibonacci number as F_n, with $F_0 = 0$; $F_1 = 1$ and $F_n = F_{n-1} + F_{n-2}$. The strong relation between the number of independent sets of graph i(G) and the Fibonacci numbers is widely known. For example, $i(P_n) = F_{n+2}$, $i(C_n) = F_{n+1} + F_{n-1}$, where P_n and C_n are the path and the cycle of n vertices, respectively. Let us consider an isolated vertex as a linear path of length zero; therefore, $i(P_1) = F_3 = 2$.

In [11,12], some properties about the sequence $\beta_{s,k} = F_s \cdot F_{k-s}$ were shown, for $k > 0$, $1 \leq s \leq k-1$. For example, the symmetrical behavior of the sequence $\beta_{k,s}$ at the position s > floor(k/2). In fact, $\beta_{k,\, floor(k/2)-j} = \beta_{k,\, floor(k/2)+j}$, if k is even, and $\beta_{k,\, floor(k/2)-j} = \beta_{k,\, floor(k/2)\, j+1}$, if k is odd and for all j such that $1 \leq j \leq floor(k/2) -2$.

Also, the sequence $\beta_{k,s}$ is increasing on the even indices of s, and it has a decreasing behavior on the odd indices of s. For example, $\beta_{k,2p} < \beta_{k,2(p+1)}$ for every $p \in \{1,2,..., floor(k/4) \}$, and all k. While, $\beta_{k,2p+1} > \beta_{t,2p+3}$ for every $p \in \{ 0,1,..., floor(k/4) -1\}$ and all k.

In Table 1, we present some of the values of the sequence $\beta_{s,k}$. Notice that different relations can be inferred when we consider the values of the table arranged like Pascal's triangle.

Table 1. The product of two Fibonaccis with complementary indices

n	F_n	$\beta_{1,k}$ Max	$\beta_{2,k}$ Min	$\beta_{3,k}$	$\beta_{4,k}$	$\beta_{5,k}$	$\beta_{6,k}$	$\beta_{7,k}$	$\beta_{8,k}$	$\beta_{9,k}$	$\beta_{10,k}$	$\beta_{11,k}$	$\beta_{12,k}$	$\beta_{13,k}$	$\beta_{14,k}$
1	1	0													
2	1	1	0												
3	2	1	1	0											
4	3	2	1	2	0										
5	5	3	2	2	3	0									
6	8	5	3	4	3	5	0								
7	13	8	5	6	6	5	8	0							
8	21	13	8	10	9	10	8	13	0						
9	34	21	13	16	15	15	16	13	21	0					
10	55	34	21	26	24	25	24	26	21	34	0				
11	89	55	34	42	39	40	40	39	42	34	55	0			
12	144	89	55	68	63	65	64	65	63	68	55	89	0		
13	233	144	89	110	102	105	104	104	105	102	110	89	144	0	
14	377	233	144	178	165	170	168	169	168	170	165	178	144	233	0

Other relevant results from [12] is that $\beta_{1,k}$=$F_1 \cdot F_{k-1}$=F_{k-1} is maximum for the series, while $\beta_{2,k}$=$F_2 \cdot F_{k-2}$=F_{k-2} is minimum for the same series at the same row(k).

Notice that the following extremal values in $\beta_{s,k}$ corresponds to $\beta_{3,k}$=$F_3 \cdot F_{k-3} = 2 \cdot F_{k-3}$ for the maximum and $\beta_{4,k}$=F_4 $\cdot F_{k-4} = 3 \cdot F_{k-4}$ for the minimum, maintaining the same row(k).

Notice that the maximum $F_1 \cdot F_{k-1} = F_{k-1}$ for the row (k) of the table results to be the minimum $F_2 \cdot F_{k-1} = F_{k-1}$ for the row (k+1). Also, the difference between the maximum and minimum in row k is $F_{k-1} - F_{k-2} = F_{k-3}$. The fact that the extremal values of $\beta_{k,s}$ are in the first two consecutive columns of Table 1, and the following extremal values are also in the following two next columns, it will have logical consequences on the topologies that represent the extremal values for the Merrifield-Simmons index on bipolygonal graphs.

Those results show new properties for $\beta_{s,k}$ that will be useful in our analysis. For example, in the following section, we show how to apply some of the properties of the serie $\beta_{s,k}$ for determining extremal topologies for bipolygonal graphs.

4 Bipolygonal Graphs

Let C_i and C_j be two polygons with the respective number of vertices i and j. A special class of graphs is formed for joining C_i and C_j via an edge e={x,y}, with $x \in V(C_i)$ and $y \in V(C_j)$, see Figure 1. We call this class of connected graph via an edge cut a bipolygonal graph, and it will be denoted by $H_{i,j}$. Especially when the polygons C_i and C_j are hexagons, $H_{i,j}$ is the primitive graph used to form chains of bipolygonal graph that represent the structure of phenylenes and bypiridines.

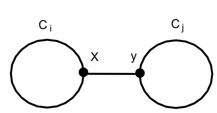


Fig. 1. A Bipolygonal Graph

Let us consider now the edge division rule: let e= {x, y} $\in$ E(G), then i(G) = i(G - e) - i(G - (N[x] $\cup$ N[y])). We show the application of this edge division rule to count the Merrifield-Simmon index on phenylenes.

Proposition 1: $i(H_{i,j}) = F_{i+1} \cdot F_{j+1} + F_{i+1} \cdot F_{j-1} + F_{i-1} \cdot F_{j+1}$

Proof. According to the edge division rule (see Figure 2):
$i(H_{i,j})=i(C_i) \cdot i(C_j)-i(P_{i-3} \cdot P_{j-3})= (F_{i+1}+F_{i-1}) \cdot (F_{j+1}+F_{j-1}) -F_{i-1} \cdot F_{j-1}$
$=F_{i+1}F_{j+1} + F_{i+1}F_{j-1} +F_{i-1}F_{j+1} + F_{i-1}F_{j-1} - F_{i-1}F_{j-1}$
$=F_{i+1}F_{j+1}+F_{i+1}F_{j-1}+F_{i-1}F_{j+1}$.

This result can be seen as $F_{i+1} \cdot (F_{j+1}+F_{j-1})+F_{i-1} \cdot F_{j+1}$ *where* $(F_{j+1}+F_{j-1})$ *represents the j-th Lucas Number.*

Let $k = i +j$, fixing $k \geq 6$, we consider the different subgraphs formed by the variations: $3 \leq i,j \leq (k-3)$. We consider that $H_{i,j}$ can be decomposed into all possible combinations of polygons C_i and C_j, keeping $i+j$ as a constant.

In Table 2, we show all possible combinations to conform C_i and C_j and fix in a constant the total number of vertices (in this case, 12 vertices). In the table, also we show how to compute their respective number of independent sets based on the above proposition. The following propositions demonstrate which combination of polygons provides the maximum and minimum independent sets for any k.

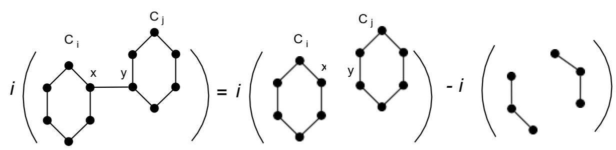


Fig. 2. A Bipolygonal Graph division edge

Theorem 1: The minimum $i(H_{i,j})=\min \{ i(H_{r,s}): r+s= k,r,s \geq 3\} = i(H_{3,k-3})$

Proof: Let $i+j=k$, $i=3$, $j=k-3$, $i(H_{3,k-3}) = F_{3+1} \cdot F_{k-3+1} + F_{3+1} \cdot F_{k-3-1} + F_{3-1} \cdot F_{k-3+1}$, *due to the proposition 1. Therefore,* $i(H_{3,k-3}) = F_4 \cdot F_{k-2} + F_4 \cdot F_{k-4} + F_2 \cdot F_{k-2} = F_4 \cdot (F_{k-2} + F_{k-4}) + F_2 \cdot F_{k-2}$.

If we assume $i>3$, *then* $i(H_{i,k-i})=F_{i+1} (F_{k-i+1} + F_{k-i-1})+F_{i-1} \cdot F_{k-i+1}$. *We have that,* $F_2 \cdot F_{k-2} < F_{i-1} \cdot F_{k-i+1}$, $\forall i > 3$, *since* $F_2 \cdot F_{k-2}$ *is the minimum in the series* $\beta_{s,k}$.

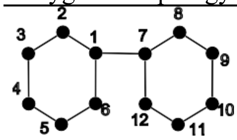
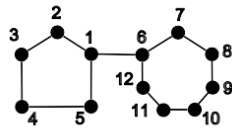
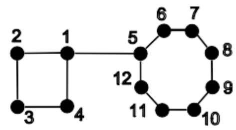
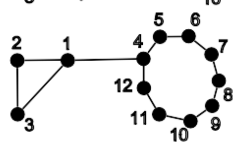
On the other hand, $F_4 \cdot (F_{k-2} + F_{k-4}) = F_4 \cdot L_{k-3}$ *and* $F_{i+1} \cdot (F_{k-i+1} + F_{k-i-1}) = F_{i+1} \cdot L_{k-i}$, *considering that* $i \geq 3$. *Thus,* $F_4 \cdot L_{k-3}<F_{i+1} \cdot L_{k-i}$, $\forall i > 3$ *because* $\beta_{s,k}$ *is increasing on the even indices of s and then* $F_4 \cdot (F_{k-2} + F_{k-4})$ *is the following minima value for any pair* $F_{i+1} \cdot (F_{k-i+1} + F_{k-i-1})$, *with* $i \geq 3$. *In this case, the minimum value of* $F_2 \cdot (F_{k-2} + F_{k-4})$ *in the row (k) does not consider because it does not represent any bipolygonal decomposition.*

Theorem 2: The maximum $i(H_{i,j})=\max \{ i(H_{r,s}): r+s= k,r,s \geq 4 \} = i(H_{4,k-4})$

Proof: Let $i+j=k$, $i=4$, $j=k-4$. *Due to the proposition 1,* $i(H_{4,k-4}) = F_{4+1} \cdot F_{k-4+1} + F_{4+1} \cdot F_{k-4-1} + F_{4-1} \cdot F_{k-4+1} =F_5 \cdot F_{k-3} + F_5 \cdot F_{k-5} + F_3 \cdot F_{k-3} =F_5 \cdot (F_{k-3} + F_{k-5}) + F_3 \cdot F_{k-3}$. *If we assume* $i>4$ *then* $i(H_{i,k-i})=F_{i+1} (F_{k-i+1} + F_{k-i-1})+F_{i-1} \cdot F_{k-i+1}$, *due to the proposition 1. We have that,* $F_3 \cdot F_{k-3} > F_{i-1} \cdot F_{k-i+1}$, *since* $F_3 \cdot F_{k-3}$ *is the following maximum value in the series* $\beta_{s,k}$ *without considering* $F_1 \cdot F_{k-1}$, *because the last value does not represent any bipolygonal decomposition.*

On the other hand, $F_5 \cdot (F_{k-3} + F_{k-5}) = F_5 \cdot L_{k-4}$ *and* $F_{i+1} \cdot (F_{k-i+1} + F_{k-i-1}) = F_{i+1} \cdot L_{k-i}$, *considering* $i \geq 4$. *Thus,* $F_5 \cdot L_{k-4}>F_{i+1} \cdot L_{k-i}$, $\forall i > 4$, *because* $\beta_{s,k}$ *is decreasing on the odd indices of s. Therefore,* $H_{4,k-4} = F_5 \cdot (F_{k-3} + F_{k-5}) + F_3 \cdot F_9$ *is the following maximal value, without considering* $F_3 \cdot (F_{k-3} + F_{k-5})$ *for any pair* $F_{i+1} \cdot (F_{k-i+1} + F_{k-i-1})$, *with* $i \geq 4$.

Table 2. Combinations of bipolygonal graphs with the same number of total vertices

Polygonal Topology	i	j	$F_{i+1}F_{j+1}+F_{i+1}F_{j-1}+F_{i-1}F_{j+1}$	I(G)
	6	6	$F_7F_7+F_7F_5+F_5F_7$	169+65+65=299
	5	7	$F_6F_8+F_6F_6+F_4F_8$	168+64+63=295
	4	8	$F_5F_9+F_5F_7+F_3F_9$	170+65+68=303
	*3*	9	$F_4F_{10}+F_4F_8+F_2F_{10}$	165+63+55=283

In Table 2, we consider that the number of vertices k for the bipolygonal graph is 12. We show that it is not required to do the explicit calculation of i(G). Instead, we need to know the values of the sequence $\beta_{s,k}$. For the analyzed instance, the extremal values are identified when the greatest variation (entropy) between the sizes of the polygons is obtained. In this case, the minimum value corresponds to $|C_j|-|C_i|= 6$, and the maximum value is given when $|C_j|-|C_i|= 4$.

When k=12, there are other different instances of polygonal chains, for example, a chain of 3 squares or a chain of 4 triangles. For those cases, different values for i(G) is obtained. For the chain of 3 squares, we have that i(G) = 287, and for a chain of 4 triangles, i(G)= 209. However, in our study, we want to keep the structure of bipolygonal graphs.

For bipolygonal graphs, we can build a series of values Hi,j for the Merrifield-Simmon index of the bipolygonal graph, where the first polygon has i vertices and the second j vertices. In this case, the serie behaves similarly to the serie $\beta_{i,j}$ from Table 1.
In Table 3, we show the values of the serie $H_{i,j}$ with his values ordered as in table 1, in the form of the triangle on the values of $H_{i,j}$.

Table 3. The Merrifield-Simon Index for bipolygonal graphs with i+j total vertices

k	Min	Max						
8	$H_{3,5}$	$H_{4,4}$	$H_{5,3}$					
9	$H_{3,6}$	$H_{4,5}$	$H_{5,4}$	$H_{6,3}$				
10	$H_{3,7}$	$H_{4,6}$	$H_{5,5}$	$H_{6,4}$	$H_{7,3}$			
11	$H_{3,8}$	$H_{4,7}$	$H_{5,6}$	$H_{6,5}$	$H_{7,4}$	$H_{8,3}$		
12	$H_{3,9}$	$H_{4,8}$	$H_{5,7}$	$H_{6,6}$	$H_{7,5}$	$H_{8,4}$	$H_{9,3}$	
13	$H_{3,10}$	$H_{4,9}$	$H_{5,8}$	$H_{6,7}$	$H_{7,6}$	$H_{8,5}$	$H_{9,4}$	$H_{10,3}$

Table 3 has the same properties shown in Table 1. In this case, $H_{i,j}$ will be an increasing series on the odd indices in i , and a decreasing series on the even indices in j. The extreme values in this series are found in the first two columns; the minimum value in $H_{3,\,k-3}$ and the maximum value in $H_{4,\,k-4}$.

5 Dynamic Trees

Let $T = (V, E)$ be a rooted tree at a vertex $v_r \in V$. We traverse T in postorder. Let $F_i = \{T_i\}, i = 1,...,n$ where F_i is a family of induced subgraphs, it is $T_i = (V_i, E_i)$, $V_i \subset V$, $E_i \subset E$, and each V_i is built as $V_i = \{v_1,... v_i\}$ of V. We associate to each vertex $v_i \in V$ a pair (α_i, β_i) with $\alpha_i = |I-v_i(T_i)|$, which means that α_i is the number of subsets in $I(T_i)$ where vi does not appear. Meanwhile, $\beta_i = |I_{vi}(T_i)|$ conveys the number of subsets in $I(T_i)$, where v_i appears. Therefore, $i(T_i) = \alpha_i + \beta_i$.

The first pair (α_1, β_1) is $(1, 1)$ since the induced subgraph $T_1 = \{v1\}$, $I(T_1) = \{\emptyset,\{v_1\}\}$ given that v_1 is a pendant vertex of T_n. The new pair $(\alpha_{i+1}, \beta_{i+1})$ is built from the previous one by a Fibonacci sequence, $(\alpha_{i+1}, \beta_{i+1}) = (\alpha_i + \beta_i, \alpha_i)$.

When a node $v_i \in V(T_n)$ has more than one child, then the Hadamard product among the $(\alpha_{ij}, \beta_{ij}), j = 1,...,k$ is formed in order to obtain (α_i, β_i). The following algorithm shows how to compute $i(T)$ for a tree T.

Let $T_n \in T(n)$ be a tree and let $v \notin V(T_n)$ be a new vertex. We consider the problem of finding where to connect v to T_n, preserving the structure of the tree, and with the aim of obtaining extremal values for the Merrifield-Simmons index on $i(T_n \cup \{\{vp, v\}\})$, with $v_p \in V(T_n)$.

We consider $v \notin V(T_n)$ as a new pendant node linked to T_n using the node $v_p \in V(Tn)$ as the father node of v, forming the new tree $T' = (T_n \cup \{\{vp, v\}\})$. Let us denote $(Tn \cup \{\{v_p, v\}\})$ as $(T_n \cup_{vp} v)$. We analyze the number of independent sets of $(T_n \cup_{vp} v)$ by using the vertex reduction rule applied on the vertex v from Eq. 1.

From Eq. (1), we see that $i(T_n)$ is an invariant since its value is independent from the place of v_p in T_n. Then, the extremal values for Eq. (1) are based only on the term $i(T_n - \{v, v_p\})$ which becomes the first objective function to optimize.

Since the node v to be added to T_n will be a leaf of T', then the father v_p of v is its unique neighbor, this is $N(v) = \{v_p\}$. Let us consider the computation of the minimum value for $i(T_n - \{v, v_p\})$. Notice that $i(T_n, \{v_p\}) = i(T_n - \{v, v_p\})$ since $v \notin V(T_n)$. In order to minimize $i(T_n, \{v_p\})$ we have that $(T_n, \{v_p\})$ would be kept as an unique connected component, and it is achieved when v_p is a leaf node of T_n.

Let $w \in V(T_n)$ the father node of v_p. We apply the vertex reduction rule on w for computing $i(T_n - \{v_p\}) = i(T_n - \{v, v_p\})$. The function $i(T_n - N[w])$ will get a minimum value when $|N[w]|$ has a maximum value, therefore w must have a maximum degree in T_n, and w must have at least one pendant vertex as a child node.

The order for holding the conditions for v_p is relevant in order to be part of the minimum of $i(T_n \cup_{vp} v)$. The main criterion is that v_p must be a leaf node of T_n. Among the possible leave nodes, the father w of v_p must have a maximal degree in T_n. Finally, if both criteria are hold by different nodes, then v_p must have a maximal eccentricity with respect to other similar internal nodes of T_n.

When a unique w T_n holds the above conditions (v_p is a leaf node whose father w in T_n is the internal node with maximum degree in T_n, and v_p has a maximal eccentricity in T_n) with respect to any other internal node in Tn, then the node v_p where v was linked, in order to minimize $i(T_n \cup_{vp} v)$, has been found in linear time.

We deal with the case where T_n has a set of nodes $W = \{v_1,..., v_r\}$ holding similar conditions. Each $v_i \in W$ has a maximal degree in T_n and it is adjacent to leaf nodes of T_n. The other case is that T_n has only nodes holding to be maximal and without leaf nodes in T_n. In those cases, it is necessary to calculate $i(T_n \cup_{vi} v)$ on each $v_i \in W$.

6 Conclusions

We have shown how properties of the sequence $\beta_{s,k}$, which represents the product between the Fibonacci numbers: F_i and F_j, can be used for the computation of the Merrifield-Simmons index on bipolygonal graphs. Our method does not require the explicit computation of the number of independent sets of the involved graphs. Instead, it is based on applying the edge division rule to decompose the initial graph. We show that the extreme values for bipolygonal graphs are found in two consecutive columns; the minimum extremal value in $\beta_{3, k-3}$ and the maximum extremal value in $\beta_{4, k-4}$.

The recognition of extremal topologies on trees is relevant in the optimization of topological invariants of chemical compounds modeled by arborescent molecular graphs [20,21,22]. We have considered here, the case of how to extend a given tree T_n through a new node v, keeping the structure of tree, and achieving extremal values for the M-S index for the new tree.

Given a tree T_n of order n, a node $v \notin V(T_n)$, and $v_p \in V(T_n)$, the M-S index of $(T \cup \{\{v_p, v\}\})$ will be minimum when v_p is a leaf node in T_n.

On the other hand, the M-S index of $T_n \cup \{\{v_p, v\}\})$ achieves a maximum value when v is linked to a node v_p with maximal degree in T_n, and v_p has a greater number of neighbors with a minimal degree in T_n.

References

1. Adegoke, K.: Some Infinite Product Identities Involving Fibonacci and Lucas Numbers. Fibonacci Q. 55 (2017) 343–351
2. Ando, S.: On a system of sequences defined by a recurrence relation. Fibonacci Q. 33 (1995) 279–282
3. Berenhaut, K. S., Magargee, E. M., Rabidoux, S. M.: Asymptotic behavior of solutions to minimum-maximum delay recurrences of higher order. In: The Fourteenth International Conference on Fibonacci Numbers and Their Applications, pp. 44--51. Instituto de Matemáticas UNAM, México (2011)
4. Bulawa, A., Lee, W.K.: Integer Values of Generating Functions for the Fibonacci and Related Sequences. Fibonacci Q. 55 (2017) 74–81
5. Cao, Y., Fuji, Z.: Extremal polygonal chains on k-matchings. MATCH Commun. Math. Comput. Chem. 60 (2008) 55–78
6. Dyer, M., Greenhill, C.: Some \#P-completeness Proofs for Colourings and Independent Sets. Research Report Series, University of Leeds (1997)
7. Deng, H.: Catacondensed Benzenoids and Phenylenes with the Extremal Thirdorder Randic Index1. MATCH Commun. Math. Comput. Chem. 64 (2010) 471–496
8. Doslic, T., Litz, M.: Matchings and Independent Sets in Polyphenylene Chains. MATCH Commun. Math. Comput. Chem. 67 (2012) 313–330
9. Edgar, T.: Extending Some Fibonacci-Lucas Relations. Fibonacci Q. 54 (2016) 79
10. Li X., Zhao, H., Gutman, I.: On the Merrifield-Simmons index of trees. MATCH Commun. Math. Comput. Chem. 54 (2005) 389–402
11. De Ita, G., Marcial, J.R., Bello, P., Contreras, M.: Linear-time Algorithms for Computing the Merrifield-Simmons Index on Polygonal Trees. MATCH Commun. Math. Comput. Chem. 79 (2018) 22–31
12. De Ita, G., Marcial, J.R., Hernández, J.A., Valdovino, R.M.: Extending Extremal Polygonal Arrays for the Merrifield-Simmons Index. In: Carrasco-Ochoa, J., Martínez-Trinidad, J., Olvera-López, J. (eds) Pattern Recognition. MCPR 2017. LNCS, vol. 10267, pp. 22--31 (2017)
13. Merrifield, R. E., Simmons, H. E.: Topological Methods in Chemistry. Wiley, New York (1989)
14. Ren, H., Zhang, F.: Double hexagonal chains with maximal Hosoya index and minimal Merrifield-Simmons index. J. Math. Chem. 42, 679--690 (2007). doi:10.1007/s10910-005-9024-2
15. Gutman, I., Li, X., Zhao, H.: On the Merrifield-Simmons index of trees. MATCH Commun. Math. Comput. Chem. 54 (2005) 389–402
16. Deng, H.: The smallest Merrifield-Simmons index of (n,n+1)-graphs. Math. Comput. Model. 49, 320--326 (2009). doi:10.1016/j.mcm.2008.06.009
17. Wagner, S., Gutman, I.: Maxima and minima of the Hosoya index and the Merrifield-Simmons index. Acta Appl. Math. 112, 323--346 (2010). doi:10.1007/s10440-010-9575-5
18. Melham, R.S.: New Identities Satisfied by Powers of Fibonacci and Lucas Numbers. Fibonacci Q. 54 (2016) 296–303
19. Zhu, Z., Li, S., Tan, L.: Tricyclic graphs with maximum Merrifield-Simmons index. Discrete Appl. Math. 158, 204--212 (2010). doi:10.1016/j.dam.2009.09.001
20. Li, X., Zhao, H., Gutman, I.: On the Merrifield-Simmons index of trees. MATCH Commun. Math. Comput. Chem. 54 (2012) 389–402
21. Lv, X., Yu, A.: The Merrifield-Simmons and Hosoya indices of trees with a given maximum degree. MATCH Commun. Math. Comput. Chem. 56 (2006) 605–616
22. Herbert, S.W.: The number of maximal independent sets in a tree. Siam J. Alg. Disc. Meth. 7 (1986) 125–130
23. Pedersen, A.S., Vestergaard, P.D.: The number of independent sets in unicyclic graphs. Discrete Appl. Math. 152, 246–256 (2005). doi:10.1016/j.dam.2005.04.002
24. Shiu, W.C.: Extremal Hosoya index and Merrifield-Simmons index of hexagonal spiders. Discret. Appl. Math. 156, 2978–2985 (2008). doi:10.1016/j.dam.2008.01.008
25. Prodinger, H., Tichy, R.F.: Fibonacci numbers of graphs. Fibonacci Q. 20 (1982) 16– 21