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Extremal graphs for the number of independent sets on polygonal chains joined by cutting edges

Guillermo De Ita Luna[1], Pedro Bello López[1], Meliza Contreras González[1], José Raymundo Marcial Romero[2]
[1]Faculty of Computer Sciences, Benemérita Universidad Autónoma de Puebla, Puebla 72570, México,
[2] Faculty of Engineering, Universidad Autónoma del Estado de México, Toluca 50000, México.
E-mails: deitaluna63@gmail.com, pedro.bello@correo.buap.mx, meliza.contreras@correo.buap.mx and jrmarcial@uaemex.mx

Abstract. We determine extremal graphs with respect to the number of independent sets for polygonal chains joined by cutting edges. We show that for any class of polygonal chains, independently of the number of sides on each polygon, the zig-zag polygonal chain has the extremal minimum value. Meanwhile, the polygonal chain at distance 2 between any two consecutive cutting edges provides the extremal maximum value. These results generalize and formalize previous ideas about phenylene chains.
To recognize those extremal topologies, extremal values for the product between two Fibonacci numbers with complementary indices are determined. The product between two Fibonacci numbers with complementary indices are also applied for recognizing extremal graphs when a path is extended with one more vertex, or when any independent subgraph is linked to the path. Our results are achieved by applying decomposition of the input graph through the vertex and edge division rules.
Keywords: Counting independent sets, Fibonacci numbers, Extremal graphs, Polygonal chains

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1 Introduction

Given a graph G = (V, E(G)), a subset S ⊆ V is called independent if for every u, v ∈ S implies that {u, v} ∈/ E(G). The corresponding counting problem on independent sets, denoted by i(G), consists of counting the number of independent sets of a graph G.

Merrifield and Simmons showed the correlation between the number of independent sets of a graph representing a chemical molecule and its boiling points. This is one of the reasons why the number of independent sets of a graph G is called the Merrifield-Simmons index of G on mathematical chemistry. Although, in the graph theory area, i(G) is also called the Fibonacci number of G.

Graphs function as representations for a multitude of systems, the structure and operation of which rely on the interconnected arrangements of their fundamental elements. Any procedure that produces a numerical value independent from a particular labeling vertex will result in a topological invariant (Doslic,2012). Many topological invariants are closely correlated with some physic chemical characteristics of the underlying compounds. It is well known that the Merrifield-Simmons (M-S) index is an important invariant for the structural chemistry Deng (2008) y Wagner & Gutman (2010). From Doslic (2012), we know that the results from M-S index have a potential use for combinatorial chemistry. The Merrifield-Simmons index stands out as one of the most favored topological indices in the realm of chemistry.

On the other hand, several works have been developed to analyze extremal values for the number of independent sets on different classes of graphs Deng (2008), Wagner & Gutman (2010), Cao & Zhang (2008), Gutman (1992), Lianzhu (1998), Zhang & Zhang

(2000). For example, the polygonal array graphs have been widely investigated and they represent a relevant area of interest in mathematical chemistry, because they have been used to study intrinsic properties of molecular graphs Pedersen (2005).

We will differentiate two classes of polygonal arrays that are commonly used to model chemical compounds. The sequence of polygons, where any consecutive pair of polygons share one edge, it will be a polygonal array. Meanwhile, a sequence of polygons where any consecutive pair of polygons are joined by one cutting edge, it will be called a polygonal chain.

Gutman (1993) analyzed extremal hexagonal arrays according to three topological invariants: Hosoya index, largest eigenvalue, and Merrifield-Simmons index. Gutman showed that the extremal topology for the maximum Merrifield-Simmons index, in the case of hexagonal arrays, is the linear hexagonal array. Meanwhile, Zhang & Zhang (2000) shown that the minimum of the M-S index on hexagonal chains is achieved by the zig-zag polyphenegraph.

The recognition of extremal graphs has been a relevant study on pattern structural recognition area. In graph theory, several works deal with the characterization of the extremal graphs concerning Hosoya and M-S indices for different graph topologies, such as trees, unicyclic graphs, and certain structures involving pentagonal and hexagonal cycles Deng (2008), Wagner & Gutman (2010), Cao & Zhang (2008), Pedersen (2005), Deng (2010), Shiu (2008), Zhu et al. (2010). For example, Ren et al. (2007) determined the minimal M-S index for double hexagonal chains. In Zhu (2010), a survey about extremal graphs for Hosoya and Merrifield-Simmons indices involving different graph topologies is considered.

A phenylene is any divalent aromatic radicals obtained from a benzene molecule by removing two hydrogen atoms. Some of those polymers, in which the basic building block is a phenylene, are called polyphenylenes. We will model the polyphenylenes by polygonal chains. Polyphenylenes are macromolecules, which comprise benzenoid aromatic nuclei directly joined to one another by C − C bonds. These materials have been known for many years, and they are modeled through polygonal chains joined by cutting edges Jones (1989). The derivatives of polyphenylenes are commonly seen chemicals, which can be used in organic synthesis, drug synthesis, heat exchanger, etc. Yang (2018).

Polyphenylenes share many structural similarities with benzenoid compounds (modeled by hexagonal arrays). Therefore, closely related classes of compounds can be efficiently modeled by both classes of graphs. However, while the study of benzenoid compounds has been followed (and in many cases preceded) by the study of benzenoid graphs, the graphs representing polyphenylene compounds remain largely unexplored Doslic et al. (2018). Our line of research is the establishment of the graph topologies for the extremal values for the M-S index for polygonal chains.

We show how the properties of the product between two Fibonacci numbers with complementary indices are useful for determining extremal graphs on a path linked to a new vertex or linked to a connected subgraph. Also, we present new results about extremal graphs for the number of independent sets on polygonal chains. Our results consider polygonal chains not uniform; it means that the polygons have different sizes and the distance between any consecutive pair of cutting edges can be variable. Our proofs do not require the explicit computation of the Merrifield-Simmons index on polygonal chains, instead the vertex and the edge division rule are applied to decompose the input graphs.

In the following section, we introduce some notation to be used as well as some related works. In section three, we present the analysis done on the product between two Fibonacci numbers with complementary indices, and we determine its extremal values. In section four, we show the analysis done for obtaining extremal values with respect to the M-S index of polygonal chains joined by cutting edges. And in section five, a note on M-S index is presented for polyphenylene dendrimers. The last section contains the conclusions.

2 Preliminaries

Let G = (V, E) be an undirected graph with a set of vertices V (or V (G)) and set of edges E (or E(G)). It is assumed that G is a simple graph if it does not have loops or parallel edges. The neighborhood of x ∈ V is the set N (x) = {y ∈ V: {x, y} ∈ E}, and its closed neighborhood is N (x)∪{x}, which is denoted by N [x]. $N_H(x)$ emphasizes the consideration of the neighbors of x, but only on the subgraph H. Therefore, NH (x) = {y ∈ V (H): {x, y} ∈ E(H)}. The degree of a vertex x in the graph G, denoted by δG(x), is $|N_G(x)|$. The degree of the graph G is $\Delta(G) = \max\{\delta_G(x): x \in V(G)\}$.

A path P_n of n vertices between the vertices v and w is a sequence $v_1v_2, \ldots, v_{n-1}v_n$ of edges such that $v_1 = v$, $v_n = w$, and $v_kv_{k+1} \in E$, for $1 \leq k < n$. A simple path is a path where $v_1, \ldots, v_{n-1}, v_n$ 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, unless the first and last vertices are identical.

For u, v ∈ V (G), d (u, v) denotes the distance between u and v in G, which is the length of the shortest path between u and v. Similarly, for e, f ∈ E(G), d (e, f) denotes the distance between the edges e and f, which is the length of the shortest path between e and f, without considering the same edges e and f.

Given a graph G = (V, E), let G′ = (V ′, E′) be a subgraph of G, then V ′ ⊆ V and E′ contains edges {v, w} ∈ E such that v ∈ V ′ and w ∈ V ′. If E′ contains every edge {v, w} ∈ E, where v ∈ V ′ and w ∈ V ′, then G′ is called the induced graph of G. A connected component of G is a maximal induced subgraph of G. Thus, a connected component of G is not a proper subgraph of any other connected subgraph of G.

An acyclic graph is a graph that does not contain cycles. The connected acyclic graphs are called trees. Let T (v) be a tree T with root vertex v. The vertices in a tree with degree equal to one are called leaves or pendant nodes, while the non-roots nodes of degree greater than one are called internal nodes of the tree. It is not difficult to infer that in a tree there is a unique path connecting any two pair of vertices. We denote by P_n, C_n, T_n, S_n and K_n to a path, a simple cycle, a tree, a star graph and a complete graph, respectively, all of them containing n vertices.

For a vertex u ∈ V (G), (G − u) denotes the graph induced by (V (G) − {u}). For an edge e ∈ E(G), (G − e) denotes the graph obtained from G by deleting the edge e, while (G\e) denotes the graph obtained by deleting e and both end-vertices.

A subset S ⊆ V is called independent, if for every u, v ∈ S implies that {u, v} ∈/ E. The corresponding counting problem on independent sets, denoted by i(G), consists of counting the number of independent sets of a graph G. Computing i(G) is a #P-complete problem for graphs G, where Δ(G) ≥ 3. The computation of i(G) remains #P-complete even if it is restricted to 3-regular graphs GreenHill (2000).

Let G = (V, E) be a molecular graph and denote by n(G, k) the number of ways in which k mutually independent vertices can be selected in G. The empty vertex set is considered an independent set, then n(G, 0) = 1 for all graphs, and n(G, 1) = |V (G)|.

Furthermore, $i(G) = \Sigma_{k\geq 0}\, n(G, k)$ is the Merrifield-Simmons index of G, which is the exact number of independent sets of G.

Some reductions rules have been useful to count combinatorial objects on graphs, particularly, the following rules are commonly used in the computation of i(G):

1. When G is formed by a list $G_1, \ldots, G_k$ of connected components, then $i(G) = \prod_{i=1}^{k} G_i$
2. Vertex reduction rule: Let v ∈ V (G), i(G) = i (G − v) + i(G − (N [v]))
3. Edge division rule: Let e = {x, y} ∈ E(G), i(G) = i (G − e) − i(G − (N [x] ∪ N [y]))

We denote the nth-Fibonacci number as F_n. The sequence of Fibonacci numbers is obtained by $F_0 = 0$, $F_1 = 1$ and $F_n = F_{n-1} + F_{n-2}$. The Fibonacci numbers and its properties have been useful in the analysis of structural compounds in the mathematical chemistry area.

Given a tree T_n with n nodes, 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 corresponds to the star: $i(S_n) = 2^{n-1} + 1$ Prodinger (1982). On the other hand, the number of independent sets for a cycle Cn with n vertices is $i(C_n) = F_{n+2} - F_{n-2}$.

Extremal values for the product of two Fibonacci numbers with complementary indices

Let P_n be a simple path with n vertices and n − 1 edges, then $i(P_n) = F_{n+2}$. Let k > 0 be a constant integer and let P_i and P_j be two disjointed simple paths with complementary indices, denoted as $(P_i \oplus P_j)$. This means that i + j = k. It is known that $i(P_i \oplus P_j) = i(P_i) \cdot i(P_j) = F_{i+2} \cdot F_{j+2}$. In De Ita, et al. (2019), the sequence $\beta_{k,s} = F_s \cdot F_{k-s}$, is introduced for all k = 2, 3, ... and $1 \leq s < k$. Some of those values are illustrated in Table (1).

The sequence $\beta_{s,k}$ is increasing on the even indices of s, and it has a decreasing behavior on the odd indices of s. For example, $\beta_{2p,k} < \beta_{2(p+1),k}$ for every p ∈ {1, 2, ..., floor(k/4)}, and all k. Meanwhile, $\beta_{2p+1,k} > \beta_{2p+3,k}$ for every p ∈ {0, 1, ...,floor(k/4)-1} and all k. For completeness, we present one of the main results of the extremal values for the sequence $\beta_{s,k}$, whose proof can be seen in [19].

Proposition 1. For any integers s with $1 \leq s < k$,

1. *if $k \geq 3$, then $\min_s \{F_s F_{k-s}\} = F_2 F_{k-2} = F_{k-2}$,*
2. *and if $k \geq 2$, then $\max_s \{F_s F_{k-s}\} = F_1 F_{k-1} = F_{k-1}$*

Table 1. Product between Fibonacci numbers with complementary indices

n	F_n	$\beta_{1,k}$ Max	$\beta_{2,k}$ Min	$\beta_{3,k}$	$\beta_{4,k}$	$\beta_{5,k}$	$\beta_{6,k}$	$\beta_{7,k}$	$\beta_{8,k}$	$\beta_{9,k}$	$\beta_{10,k}$	$\beta_{11,k}$	$\beta_{12,k}$	$\beta_{13,k}$
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

According to the above proposition, if we fix a row (k), the value $\beta_{1,k} = F_1 \cdot F_{k-1} = F_{k-1}$ is the maximum value for the series in the row k, while $\beta_{2,k} = F_2 \cdot F_{k-2} = F_{k-2}$ is the minimum for the same series in the same row k. The remaining values of the series are between these values: $F_{k-2} < F_s \cdot F_{k-s} < F_{k-1}$, $\forall s = 3, \ldots, k-3$. The difference between the maximum and the minimum in the row k is the following Fibonacci number: $F_{k-1} - F_{k-2} = F_{k-3}$. Notice that by maintaining the same row k, the following extremal values in $\beta_{s,k}$ correspond to $\beta_{3,k} = F_3 \cdot F_{k-3}$ for the maximum, and $\beta_{4,k} = F_4 \cdot F_{k-4}$ for the minimum. Notice that the maximum value for the row k results to be the minimum for the next row k + 1. The fact that the extremal values of $\beta_{k,s}$ are in the first two consecutive columns of the Table (1), and the following extremal values are 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 different topology graphs, as we show in the following sections.

3 Extremal topologies for the Merrifield-Simmons index on basic variations of a path

Let P_n be a simple path with n vertices, $P_n : v_1v_2, \ldots, v_{n-1}v_n$. And let $u \in / V(P_n)$ be a vertex independent from P_n. We want to determine where to connect u to P_n via a cutting edge to obtain extremal configurations for $i(P_n \cup u)$. For example, let us assume that u is linked to a vertex $v_k \in P_n$, $1 \leq k \leq n$, making an additional edge: $\{v_k, u\}$. We denote the resulting graph as $(P_n \cup_{vk} u)$.

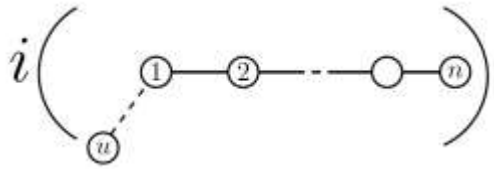


Figure. 1. Minimum topology for the M-S index for $i(P_n \cup_{vk} u)$.

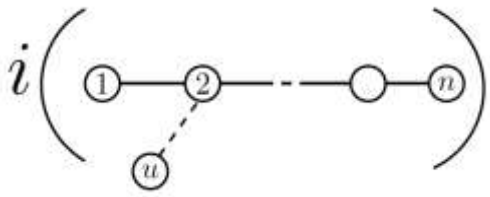


Figure. 2. Maximum topology for the M-S index for $i(P_n \cup_{vk} u)$.

Lemma 1. i($P_n \cup_{vk} u$) is minimum (maximum) for k = 1 (k = 2).

Proof. We apply the vertex reduction rule on u to compute i($P_n \cup_{vk} u$).

$$i(P_n \cup_{vk} u) = i(P_n) + i(P_n - \{vk, u\}) = i(P_n) + i(P_{k-1}P_{n-k})$$
$$= F_{n+2} + F_{k+1} \cdot F_{n-k+2}. \quad (1)$$

The term F_{n+2} in eq. 1 is invariant, because it does not depend on the place where u was linked to P_n. Therefore, the extremal values for i($P_n \cup_{vk} u$) only depend on the term $F_{k+1} \cdot F_{n-k+2}$, when it has the maximum or the minimum value.

According to proposition 1, the minimum value for the series $\beta_{k+1,n+3} = F_{k+1} \cdot F_{n+3-\{k+1\}}$ is obtained when $F_{k+1} = F_2 = 1$, meaning that k = 1. In this case, ($P_n \cup_{v1} u$) = P_{n+1} and the position to insert u to P_n for minimizing i($P_n \cup_{vk} u$), is in any endpoint of the path, as it is illustrated in Figure 1.

On the other hand, according to proposition 1, the maximum value for the series $\beta_{k+1,n+3} = F_{k+1} \cdot F_{n+3-\{k+1\}}$ is obtained when $F_{k+1} = F_1 = 1$. However, in this case k = 0, and there is no vertex $v_k \in P_n$ that becomes the father of u. Thus, the following maximal value is obtained when $F_{k+1} = F_3 = 2$, meaning that k = 2. In this case, ($P_n \cup_{v2} u$) is a path where its second node has the leaf u. Thus, the position to link u to P_n to maximize i($P_n \cup_{vk} u$) is in the second vertex of P_n, as it is illustrated in Figure 2.

□

Let us consider again a simple path P_n of n vertices $P_n : v_1v_2, \ldots, v_{n-1}v_n$. And let H be any connected subgraph that is independent from P_n, then (V (P_n) ∩ V (H)) =∅. Let u be an arbitrary vertex from V (H). Consider a new connected component ($P_n \cup_e$ H), which is formed by linking Pn to H via a cutting edge e = {v_k, u} with $v_k \in$ V (P_n), u ∈ V (H), as it is illustrated in Figure 3.

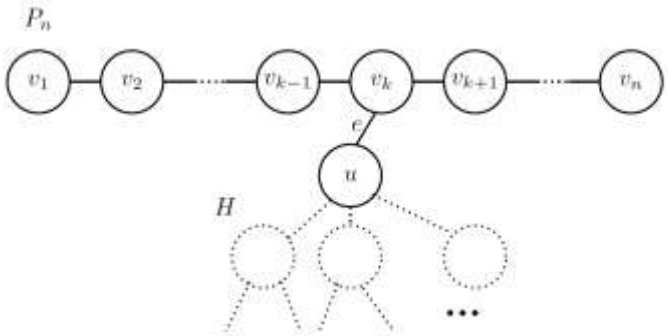


Figure 3. $P_n \cup_e$ H, with e = {v_k, u}, u ∈ V (H), $v_k \in$ V (P_n), (V (P_n) ∩ V (H)) = ∅).

Lemma 2. i($P_n \cup_e$ H) has a maximum (minimum) value when e = {v_2, u} (e = {v_1, u}).

Proof. I($P_n \cup_e H$) is computed based on the division vertex u ∈ H, which is one endpoint of the cutting edge e = {v_k, u}, $v_k \in V(P_n)$, u ∈ V (H).

$$i(P_n \cup_e H) = i((P_n \cup_e H) - \{u\}) + i((P_n \cup_e H) - N[u])$$
$$= i(P_n) \cdot i(H - \{u\}) + i(P_{k-1}) \cdot i(P_{n-k}) \cdot i(H - N[u]) \quad (2)$$

Notice that only the term $i(P_{k-1}) \cdot i(P_{n-k})$ in eq. 2 depends on the value of k, while the remaining terms in eq. 2 are invariant values that do not depend from k. For example, i(H − {u}) and i(H − N [u]) are constant values with respect to the selected vertex v_k. Therefore, the maximum and minimum values for i($P_n \cup_e H$) only depend on the maximum and minimum values for $i(P_{k-1}) \cdot i(P_{n-k})$.

Notice that $i(P_{k-1}) \cdot i(P_{n-k}) = F_{k+1} \cdot F_{n-k+2}$, and this is the product between two Fibonacci numbers with complementary indices.

In this case, the upper index is k + 1 + n − k + 2 = n + 3. By proposition 1, $F_{k+1} \cdot F_{n-k+2}$ is minimum for $F_2 \cdot F_{n+3-(2)}$, implying that k = 1. Similarly, $F_{k+1} \cdot F_{n-k+2}$ is maximum when $F_{k+1} = F_1$, and for this case k = 0. However, P_n starts in v_1; therefore, the index for the following maximal in the product between two Fibonacci's is obtained when $F_{k+1} = F_3$, implying that k = 2.

□

Notice that the maximum and minimum values for $i(P_n \cup_e H)$, $e = \{v_k, u\}$, $v_k \in V(P_n)$, $u \in V(H)$ depends only on the position v_k in P_n, and both the topology of the subgraph H and the selected vertex $u \in V(H)$ are not significant.

Counting independent sets on basic variations of an initial graph

With the daily use of technology and the resulting low school performance, Smart learning systems have been chosen, which allow to know the strengths and weaknesses of the students, and from this with the use of artificial intelligence, to propose improvements so that the learning of the students increases considerably in a safe way.

The following Lemmas and Corollary will be useful for our analysis. They show that given an initial graph G = (V, E), if new edges are added to E(G), then i(G) is decreasing. Meanwhile, if new vertices are added to V (G), then i(G) is increasing, even if the new vertices are connected to all original $v \in V(G)$.

Lemma 3. Let G = (V, E) be an undirected graph, let $x, y \in V(G)$, and $e = \{x, y\}$ not $\in E(G)$, then $i(G) > i(G \cup e)$.

Proof. Let $Se = \{S \in I(G): x, y \in S\}$ be the independent sets in G containing the two vertices $x, y \in V$. $|S_e| > 0$ since at least the set $\{x, y\} \in Se$, because e not $\in E(G)$. We have that $i(G \cup e) = i(G) - |S_e|$, then $i(G) > i(G \cup e)$.

□

Lemma 4. Let G = (V, E) be an undirected graph, and let x not $\in V$. Let $G_1 = G \cup \{\{x, v\}: \forall v \in V\}$, then $i(G_1) = i(G) + 1$.

Proof. $I(G_1) = I(G) \cup \{\{x\}\}$, since there are no more independent sets including x and any other vertex from V. Therefore, $i(G_1) = i(G) + 1$.

□

Corollary 3.1. Let G = (V, E) be an undirected graph, and let x, v be two vertices such that x not $\in V$, $v \in V$. Let $G_1 = G \cup \{\{x, v\}\}$, then $i(G_1) > i(G)$.

Proof. According to the previous lemma, $i(G_1) = i(G) + 1$ if there are no more edges between x and any other vertex $v \in V$. If any edge $\{v, x\}$ is omitted in $E(G_1)$, then G_1 is even greater than $i(G) + 1$. In any case, $i(G_1) > i(G)$.

□

Thus, we can summarize some results about counting independent sets in a graph G when additional vertices or additional edges are joined:

1. If v is an island that is adding to G, then: $i(G \cup \{v\}) = i(G) * 2$.

2. If v is joined to G as a vertex all connected in G, then $i(G \cup \{v\}) = i(G) + 1$.

3. If v is joined to G as a vertex all connected in $(G-\{u\})$, $u \in V(G)$, then $i(G \cup \{v\}) = i(G) + 2$. Generally, joining any vertex v to G increases the value $i(G \cup \{v\})$ with respect to i(G).

4. Let $e = \{x, y\}$, $x, y \in V(G)$ such that e not $\in E(G)$, then $i(G) > i(G \cup e)$. Then, the addition of new edges to G decreases the value $i(G \cup e)$ with respect to i(G).

4 Extremal topologies for polygonal chains

With the daily use of technology and the resulting low school performance, Smart learning systems have been chosen, which

allow to know the strengths and weaknesses of the students, and from this with the use of artificial intelligence, to propose improvements so that the learning of the students increases considerably in a safe way.

A polygon (also called a polygonal graph) is a simple cycle graph. Therefore, a cycle graph C_k of length k represents a polygon of k sides, which forms a k-gon. The way that two k-gons are joined (via a common vertex, a common edge or through a cutting edge) defines different classes of polygonal chemical compounds.

Let us consider a polygonal chain H_n as a sequence of n polygons h_i, i = 1, . . ., n, where each consecutive pair of polygons $h_i \cdot h_{i+1}$ are joined by a cutting edge $e_i = \{x_i, y_i\}$, i = 1, . . . , n − 1 where $x_i \in V(h_i)$, $y_i \in V(h_{i+1})$. This means that $H_n = h_1 \cup_{e1} h_2 \cup_{e2} \ldots \cup_{en-2} h_{n-1} \cup_{en-1} h_n$. Note that in this case, $(V(h_i) \cap V(h_j)) = \emptyset$ for $i \neq j$, i, j = 1, . . . , n. Also, that $\delta(x_i) = \delta(y_i) = 3$, i = 1, . . . , n − 1, while $\forall x \in (V(H_n) - \cup^{n-1}_{i=1} V(e_i))$, $\delta(x) = 2$. We call this class of graphs as a polygonal chain joined by cutting edges (see Figure 3). When each polygon in the chain H_n of n polygons is a k-gons, then we say that H_n is a regular polygonal chain, or simply a polygonal chain denoted as $H_{k,n}$.

In a polygonal chain H_n, the polygons forming the chain can have any length, including hexagons. Therefore, when we depict polygonal chains, we will draw cycles to refer to polygons with an unknown number of sides. In fact, a polygonal chain might contain polygons with different lengths, which would make not uniform chains of polygons joined by cutting edges. This class of graphs are also known as ideal H_n:

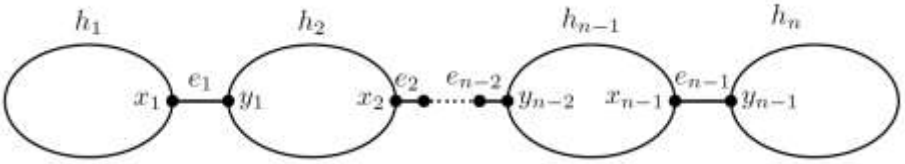


Figure. 4. A polygonal chain joined by cutting edges.

chains (or freely jointed chains). In a polygonal chain H_n with $n \geq 2$, there are two end-polygons, h_1 and h_n, while $h_2, \ldots, h_{n-1}$ are the internal polygons of the chain.

The phenylenes are chemical compounds modeled by hexagonal chains. Similarly, if the graph obtained by contracting every hexagon into a vertex in a phenylene system is a path, then such graph is called a polyphenylene chain Yang (2018). Each polyphenylene chain contains exactly two hexagons with only one cutting edge, which are called terminal hexagons, while the other hexagons are called internal. From now on, we will consider a chain of polygons joined by cutting edges, where each polygon of the chain can have a different length to the rest of the polygons on the chain, see e.g. Figure 4.

Polyphenylenes make an important class of compounds that serve as precursors to many scientifically and commercially interesting materials, such as polyphenylene oxide and polyphenylene sulfide. 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 Gutman & Furtula (2012). The major interest in polyphenylenes stemmed from their characteristic thermal and thermo-oxidative stabilities. A recent interest in them has arisen from the finding that one member of this class of polymers, poly (p-phenylene) (PPP; 1), can be transformed from an electrical insulator into an electrical conductor upon doping with electron acceptors or donors Jones (1989).

On the other hand, an ideal chain is the simplest model to describe polymers, such as nucleic acids and proteins. It only assumes a polymer as a random walk and neglects any kind of interactions among monomers. Although it is simple, its generality gives insight about the physics of polymers. In this model, monomers are rigid rods of a fixed length, and their orientation is completely independent from the orientations and positions of neighboring monomers to the extent that two monomers can coexist in the same place. In some cases, the monomer has a physical interpretation, such as an amino acid in a polypeptide. In other cases, a monomer is simply a segment of the polymer that can be modeled as a discrete, freely jointed unit Rippe (2001).

In this section, we will determine the extremal graphs regarding the Merrifield- Simmons index of a polygonal chain H_n where each pair of consecutive polygons is joined by a cutting edge, i.e. $Hn = h_1 \cup_{e1} h_2 \cdot \cdot \cdot \cup_{en-1} h_n$. Let us consider a new polygon h independent from H_n. h is linked as the n + 1 polygon via a new cutting edge $e = \{u, v\}$, $u \in V(h_n)$, $v \in V(h)$. That new polygonal chain is denoted as $(H_n \cup_{eh})$. Let us consider $k = |h_n|$, $j = |h|$. $d = d(e_{n-1}, e)$ is the distance between the last cutting edge e_{n-1} in H_n and the new cutting edge e. The extremal graphs for $i(H_n \cup_e h)$ are expressed by the following theorem.

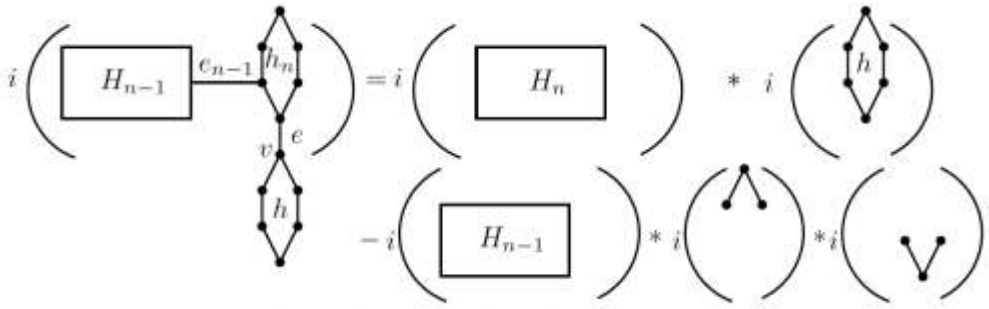


Figure. 5. Computation of i($H_n \cup_e h$), for d = d(e_{n-1}, e) = 1.

Theorem 1. i($H_n \cup_e h$) has a maximum (minimum) value for the distance d(e_{n-1}, e) = 2 (d(e_{n-1}, e) = 1).

Proof. For this demonstration, the computation of i($H_n \cup_e h$) is performed via the edge division rule on e.

$$i(H_n \cup_e h) = i(H_n) \cdot i(h) - i(H_n - N[u]) \cdot i(h - N[v]) \quad (3)$$

Notice that the term $i(H_n) \cdot i(h)$ is an invariant that does not depend on the distance d between e_{n-1} and e, neither the size of the polygons in H_n. Similarly, the factor $i(h - N[v])$ decomposes h by deleting 3 vertices from h, forming a path P_{j-3} with j−3 vertices. Therefore, $i(h-N[v]) = i(P_{j-3}) = F_{j-1}$, which results in a constant value that does not depend on the distance d.

The unique term in eq. 3, which depends on the distance d between e_{n-1} and e, is $i(H_n - N[u])$. Let us analyze the different values for this term with respect to the different values for d by considering that $h_n = v_1 - v_2 - \cdots - v_k - v_1$.

If d = 1, and $i(H_n - N[u])$ is computed in eq. 3, then $i(H_n - N[u]) = i(H_{n-1}) \cdot i(P_{k-3}) = i(H_{n-1}) \cdot F_{k-1}$, since the polygon hn is disconnected from H_n. This forms H_{n-1} and an independent path P_{k-3} with k − 3 vertices, as it is illustrated in Figure 5.

If d = 2, and the term $i(H_n - N[u])$ is computed in eq. 3, then $i(H_n - (N[u])) = i(H_{n-1} \cup_{v1} P_{k-3})$, since the polygon h_n lost 3 vertices, however, it continues as a path linked to the last polygon of H_{n-1}, as it is illustrated in Figure. 6.

If d = 3, and $i(H_n - N[u])$ is computed in eq. 3, then $i(H_n - (N[u])) = i(H_{n-1} \cup_{v2} P_{k-3})$, since the polygon hn lost 3 vertices, but it continues as a path linked to the last polygon of H_{n-1}, as it is illustrated in Figure 7. In general, considering a distance d between e_{n-1} and e, and by applying the edge reduction rule one, when $i(H_n - N[u])$ is computed, then we obtain $i(H_n - (N[u])) = i(H_{n-1} \cup_{vd-1} P_{k-3})$, since the polygon h_n lost 3 vertices. Nevertheless, it continues as a path linked to the last polygon of H_{n-1} via the edge cutting e_{n-1}.

On the other hand, the graph $(H_{n-1} \cup_{vd-1} P_{k-3})$ is the exact topology analyzed in lemma 2, where the minimum (maximum) for $i(H_{n-1} \cup_{vd-1} P_{k-3})$ is obtained when $d - 1 = 1 (d - 1 = 2)$. If h is linked at distance 2 (d = 2), then the minimum value for $i(H_{n-1} \cup_{vr-1} P_{k-3})$ is obtained. And the maximum value for $i(H_{n-1} \cup_{vd-1} P_{k-3})$ is obtained when $v_{d-1} = v_2$. This means that the distance $d = (e_{n-1}, e) = 3$.

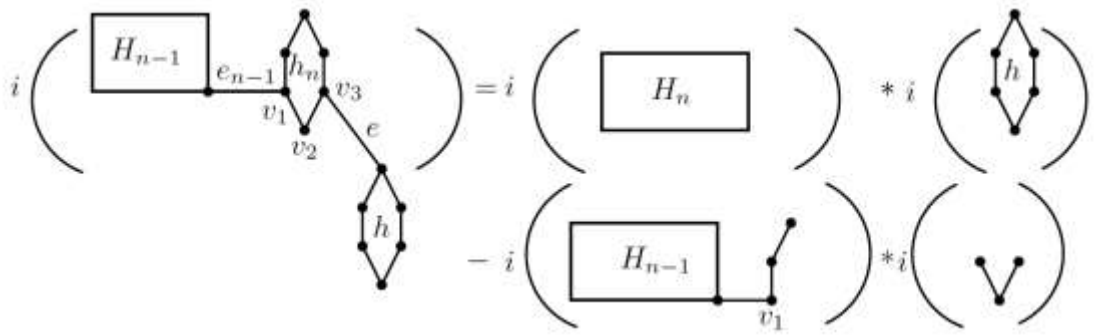


Figure. 6. Computation of $i(H_n \cup_e h)$, for $d = d(e_{n-1}, e) = 2$.

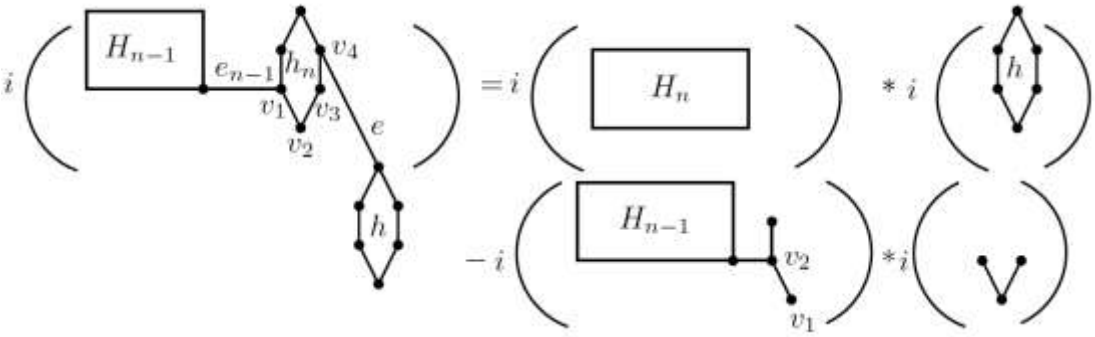


Figure. 7. Computation of $i(H_n \cup_e h)$, for $d = d(e_{n-1}, e) = 3$

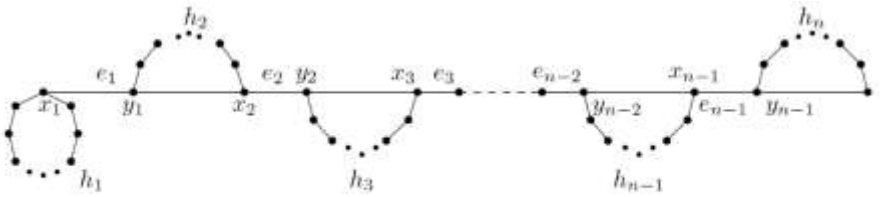
Thus, the extremal minimum topology for $i(H_n - N[u])$ is achieved when $d = d(e_{n-1}, e) = 2$. As this term appears subtracting in eq. 3, then the union of h to h_n at distance 2 between the edges e_{n-1} and e makes the maximum value for $i(H_n \cup_e h)$. Although $i(H_{n-1} \cup_{vd-1} P_{k-3})$ has a maximum value when $d = 3$, it occurs only if P_{k-3} continues connected to H_{n-1} while $i(H_n \cup_e h)$ is being computed. However, the subgraph $G' = (H_{n-1} \cdot P_{k-3})$ is reduced from $G'' = (H_{n-1} \cup_{vd-1} P_{k-3})$, if the cutting edge that links h_{n-1} to P_{k-3} is deleted. Then $G' = (G'' - \{e_{n-1}\})$ and by lemma 3, $i(G') > i(G'')$ holds.

Since G'' represents the maximum topology for all distance $d > 2$, while G' is the subgraph obtained when the distance between e_{n-1} and e is one in $i(H_n \cup_e h)$. Therefore, the maximum value for $i(H_n - (N[u]))$ is obtained at distance $d = 1$. As this term appears subtracting in eq. 3, then $i(H_n \cup_e h)$ achieves a minimum value when h is linked to h_n at distance one between cutting edges e_{n-1} and e. In this way, we obtain the extremal graphs for $i(H_n \cup_e h)$.

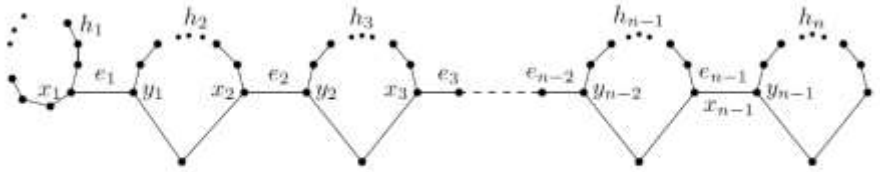
□

Notice that in the previous proof, the values $j = |h|$ and $k = |h_n|$ are not relevant as long as $j, k > 4$. This means that the extremal graphs are kept regardless of the size of the involved polygons (while they have more than four sides) in the chain H_n.

Let us consider that H_n is built iteratively. This means, that h_1 is joined to h_2, after h_2 is joined to h_3, and so on. Under the restriction that $d(e_i, e_{i+1}) > 0$, $i = 1, \ldots, n-2$. If distance one is kept between two consecutive polygons, then the minimum extremal topology for $i(H_n)$ is formed. In this case, H_n corresponds to the polygonal chain that maintains distance one between any two consecutive cutting edges, which is known as the zig-zag polygonal chain.



a) The Zig-Zag chain is the minimum extremal topology.



b) Maximum extremal topology is obtained when $d(e_i, e_{i+1}) = 2, i = 1, 2, ..., n-2$.

Figure 8. Extremal topologies for polygonal chains.

Theorem 1 shows that the minimum polygonal chain corresponds to the well-known zig-zag chain. In a zig-zag chain, the induced subgraph from Hn, which is derived by the vertices of the cutting edges, forms a simple path. Thus, for polygonal chains joined by cutting edges, the minimum extremal topology is the zig-zag chain.

Also, considering that the chain H_n is built iteratively, starting from the polygon h_1, and joining it to h_2, and so on, holding at distance two between any pair of consecutive polygons. In each block of the chain, the topology formed corresponds to the maximum extremal topology for $i(H_j)$, $j = 2, \ldots, n$. Thus, under the restriction $d(e_i, e_{i+1}) > 0$, $i = 1, \ldots, n-2$, the maximum extremal topology for $i(H_n)$ corresponds to the polygonal chain that maintains distance two between any two consecutive cutting edges in the polygonal chain.

The minimum and maximum extremal graphs for polygonal chains joined by cutting edges are depicted in Figures (8a) and (8b). Our last theorem generalizes the results obtained in the polyphenylene chains literature.

The results by Doslic et al. (2018) are consistent with our results when only phenylenes are considered as the polygons forming the chain. Doslic shown that the Ortopolyphenylenes chains (those whose distance between cutting edges is one) are the minimum extremal topologies. On the other hand, the maximum extremal graphs are formed by Meta-polyphenylenes chains (those whose distance between cutting edges is two). Therefore, the Para-polyphenylenes chains (those whose distance between cutting edges is three) have a Merrifield-Simmons index between the previous two cases. Those results by Doslic et al. (2018) about polyphenylene chains are derived from our theorem 1 as a special case, when just hexagons are considered in order to form polygonal chains.

Furthermore, Theorem 1 is held regardless of the length of the polygons in the chain, or if the chain has polygons with different lengths (is uniform or not). In summary, considering the Merrifield-Simmons index of polygonal chains, distance one between each pair of consecutive cutting edges provides the minimum extremal topology of the polygonal chains. Meanwhile, distance two between each pair of consecutive cutting edges provides the maximum extremal topology of the polygonal chains.

If we consider distance zero between cutting edges in each consecutive pair of polygons, then another maximum extremal topology is obtained among all chains with polygons joined by cutting edges. If we consider the vertex joining different cutting edges and by applying the vertex reduction on that vertex, then a maximum number of edges of the chain are deleted. That vertex has a neighborhood containing vertices with maximum degree, and it disjoints the graph into a maximum number of connected components in the chain.

5 Conclusions

We have shown how properties of the product between two Fibonacci numbers with complementary indices are useful for determining extremal graphs on paths and polygonal chains joined by cutting edges, with respect to the Merrifield-Simmons index. We show that given a path $P_n : v_1, v_2, \ldots, v_n$ with n vertices, and a new vertex v to be linked to P_n; (P_{n+1}) and $(P_n \cup_{v2} v)$ are the minimum and maximum topologies for the Merrifield-Simmons index, respectively. Similar results are obtained if instead of only one vertex v, a subgraph H with an identified vertex v is considered for computing $(P_n \cup_{vk,v} H)$.

In this article, according to the Merrifield-Simmons index, we have determined extremal graphs for polygonal chains joined by cutting edges. We have shown that the zig-zag polygonal chain has the extremal minimum value. Meanwhile, polygonal chains at distance 2 between any two consecutive cutting edges provide the extremal maximum value. In the proofs for determining those extremal topologies, the number of sides of the polygons (while they have more than four sides) is not relevant. Our result generalizes previous results obtained for Polyphenylene Chains.

Our method does not require the explicit computation of the Merrifield-Simmons index of the involved graphs. Instead, it is based on the application of the vertex and edge division rule to decompose the input graphs.

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