

Extending Extremal Polygonal Arrays for the Merrifield-Simmons Index

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Abstract. 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. For example, to determine the Merrifield-Simmons index of a polygonal array A_n that is the number of independent sets of that graph, denoted as $i(A_n)$.

In this paper we consider the problem of extending an initial polygonal array A_n adding a new polygon p to form A_{n+1} , for minimizing or maximizing the Merrifield-Simmons index $i(A_{n+1}) = i(A_n \cup p)$. Our method does not require to compute $i(A_n)$ or $i(A_n \cup p)$, explicitly.

Keywords: Counting the number of independent sets · Enumerative algorithms · Efficient counting · Merrifield-Simmons index

1 Introduction

Counting problems are not only mathematically interesting, but also they arise in many applications. Regarding hard counting problems, the computation of the number of independent sets of a graph G , denoted as $i(G)$, has been a key in determining the frontier between efficient and intractable counting problems.

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. In addition, it is also of great importance to recognize substructures of those compounds and learn messages from the graphic model by clear elucidation of their structures and properties [6].

There are several works analyzing extremal values for the number of independent sets (known in mathematical chemistry as the Merrifield-Simmons index) on chain graphs [6, 7]. Merrifield and Simmons showed the correlation between $i(G)$ and boiling points on polygonal chain graphs that represent chemical molecules. This index is a typical example of an invariant graph used in mathematical chemistry for quantifying relevant details of molecular structures.

In 1993, Gutman discussed the extremal hexagonal chains according to three topological invariants: Hosoya index, largest eigenvalue and Merrifield-Simmons index. His work greatly stimulated the study of extremal polygonal chains.

On his seminal paper [3], Gutman showed extremal linear chains for Merrifield index in the particular case of hexagonal chains. He conjectured that the chain with the smallest Merrifield-Simmons index is unique and it corresponds to the zig-zag polyphenegraph.

L.Z. Zhang et al. [4,5] showed Gutman's conjecture. They showed that the minimum value for the Merrifield-Simmons index is achieved by the zig-zag polyphenegraph. Later on, Cao et al. [2] showed extremal polygonal chains for k -matchings (Hosoya index), considering the topology of polygonal arrays that provide maximum as well as minimum values for the Hosoya index. Their demonstrations are based on the use of the Z -polynomial (Z -counting polynomial).

The previous mentioned works are concerned to hexagonal chains, or to the Hosoya index. We consider in this paper, results for the Merrifield-Simmons index for any kind of polygonal arrays. We consider the problem of extending a polygonal array A by adding a new polygon p , preserving the structure of polygonal arrays and such that $i(A \cup p)$ is maximum. Instead of computing the Z -polynomial for the Merrifield-Simmons index as Cao et al. [2] suggested, our proofs are based on properties that are derived from the product between Fibonacci's numbers with complementary indexes values. In fact, our method does not require compute $i(G)$ explicitly, and it can be adapted to compute other intrinsic properties on molecular graphs.

2 Polygonal Chains

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, $n(G, 0) = 1$ and $n(G, 1) = |V(G)|$, for all graph 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 polygonal chain is a graph $P_{k,t}$ obtained by identifying a finite number of t congruent regular polygons such that each basic polygon, except the first and the last one, is adjacent to exactly two basic polygons. When each polygon in $P_{k,t}$ has the same number of k nodes, then $P_{k,t}$ becomes a linear array of t k -gons. A special class of polygonal chains is the class of hexagonal chains, which are chains formed by n 6-gons. Hexagonal systems play an important role in mathematical chemistry as they are natural representations of catacondensed benzenoid hydrocarbons.

The propensity of carbon atoms to form compounds, made of hexagonal arrays fused along the edges gives a relevant importance to the study of chemical properties of benzenoid hydrocarbons. Those graphs have been widely investigated and represent a relevant area of interest in mathematical chemistry, since it is used for quantifying relevant details of the molecular structure of the benzenoid hydrocarbons [1,6].

Let $H_n = h_1 h_2 \cdots h_n$ be a polygonal chain with n basic polygons, where each h_i and h_{i+1} have exactly one common edge $e_i, i = 1, 2, \dots, n - 1$. A polygonal chain with at least two polygons has two end-polygons, h_1 and h_n , while h_2, \dots, h_{n-1} are the internal polygons of the chain. In a polygonal chain, each vertex has degree either 2 or 3. The vertices of degree 3 are exactly the end points of the common edges between two consecutive polygons.

The distance $d_G(x; y)$ from a vertex x to another vertex y is the minimum number of edges in an $x - y$ path of G . Similarly, we define the distance between two edges e_1, e_2 on the graph G as the minimum number of edges in an $e_1 - e_2$ path of G .

Let H_n be a polygonal chain with n basic polygons joined by one common edge between two consecutive basic polygons. If for each pair of consecutive joining edges e_i and e_{i+1} of the polygonal chain it holds that $d_{H_n}(e_i, e_{i+1}) = 2$ then H_n is known as a linear polygonal chain (L_n), and if $d_{H_n}(e_i, e_{i+1}) = 1$ for each pair of consecutive common edges, then H_n is known as a zig-zag polygonal chain (Z_n), see Fig. 1 for an example.

In recent years, several works have been done for determining the extremal graphs corresponding to the Hosoya and Merrifield-Simmons indexes [2, 6, 7]. For many graph classes that have been studied so far, the graph that minimizes the Merrifield-Simmons index is also the one that maximizes the Hosoya index, and vice versa, although its relation is still not totally understood.



Fig. 1. Example of a zig-zag octagonal chain

3 Fibonacci Properties to Compute Indices of Polygonal Chains

It is known that for any simple path P_n of size n (P_n has n vertices), P_n fulfills $i(P_n) = F_{n+2}$, where F_n is the n th-Fibonacci number with initial values $F_0 = 0, F_1 = 1$.

Let us consider an isolated vertex as a linear path of size 1, since in this way $i(P_1) = F_3 = 2$. Thus, the size of any simple path is the number of vertices in it. Let $k > 0$ be a constant integer and let P_i and P_j be two disjoint simple paths, such that $i + j = k$. It is known that $i(P_i \cdot P_j) = i(P_i) \cdot i(P_j) = F_{i+2} \cdot F_{j+2}$. We want to determine for which pair (i, j) , $i, j \geq 2$, the value of $i(P_i) \cdot i(P_j)$ is maximum when $j + i = k$, for any $k > 0$ constant.

We apply Binet's formula to state the computation of Fibonacci numbers, i.e. $F_t = \frac{a^t - b^t}{a - b}$, where $a = \left(\frac{1 + \sqrt{5}}{2}\right)$ and $b = \left(\frac{1 - \sqrt{5}}{2}\right)$ are roots of the polynomial $r^2 - r - 1 = 0$. Furthermore, $a + b = 1$ and $ab = -1$.

Let us define the sequence $\beta_{t,s}$, with $t \geq 1$ and $t \geq s \geq 1$ as follows

$$\beta_{t,s} = F_s F_{t-s} \quad (1)$$

We firstly show that the sequence $\beta_{t,s}$ becomes symmetric when $s > \lfloor \frac{t}{2} \rfloor$,

Lemma 1. *For all j , such that $1 \leq j \leq \lfloor \frac{t}{2} \rfloor - 2$, the sequence $\beta_{t,s}$ satisfies the following*

1. $\beta_{t, \lfloor \frac{t}{2} \rfloor - j} = \beta_{t, \lfloor \frac{t}{2} \rfloor + j}$ if t is even,
2. $\beta_{t, \lfloor \frac{t}{2} \rfloor - j} = \beta_{t, \lfloor \frac{t}{2} \rfloor + j + 1}$ if t is odd,

Proof. From Eq. (1) we have

$$\begin{aligned} (a-b)^2 \beta_{t, \lfloor \frac{t}{2} \rfloor - j} &= \left(a^{\lfloor \frac{t}{2} \rfloor - j} - b^{\lfloor \frac{t}{2} \rfloor - j} \right) \left(a^{t - \lfloor \frac{t}{2} \rfloor + j} - b^{t - \lfloor \frac{t}{2} \rfloor + j} \right) \\ &= a^t - a^{\lfloor \frac{t}{2} \rfloor - j} b^{t - \lfloor \frac{t}{2} \rfloor + j} - a^{t - \lfloor \frac{t}{2} \rfloor + j} b^{\lfloor \frac{t}{2} \rfloor - j} + b^t \end{aligned}$$

$$(a-b)^2 \beta_{t, \lfloor \frac{t}{2} \rfloor + j} = a^t - a^{\lfloor \frac{t}{2} \rfloor + j} b^{t - \lfloor \frac{t}{2} \rfloor - j} - a^{t - \lfloor \frac{t}{2} \rfloor - j} b^{\lfloor \frac{t}{2} \rfloor + j} + b^t$$

Thus,

$$\begin{aligned} (a-b)^2 \beta_{t, \lfloor \frac{t}{2} \rfloor - j} &= a^t - a^{\lfloor \frac{t}{2} \rfloor - j} b^{t - \lfloor \frac{t}{2} \rfloor + j} - a^{t - \lfloor \frac{t}{2} \rfloor + j} b^{\lfloor \frac{t}{2} \rfloor - j} + b^t \\ &\quad - a^{\lfloor \frac{t}{2} \rfloor + j} b^{t - \lfloor \frac{t}{2} \rfloor - j} - a^{t - \lfloor \frac{t}{2} \rfloor - j} b^{\lfloor \frac{t}{2} \rfloor + j} \\ &\quad + a^{\lfloor \frac{t}{2} \rfloor + j} b^{t - \lfloor \frac{t}{2} \rfloor - j} + a^{t - \lfloor \frac{t}{2} \rfloor - j} b^{\lfloor \frac{t}{2} \rfloor + j} \\ &= (a-b)^2 \beta_{t, \lfloor \frac{t}{2} \rfloor + j} + a^{\lfloor \frac{t}{2} \rfloor + j} b^{t - \lfloor \frac{t}{2} \rfloor - j} + a^{t - \lfloor \frac{t}{2} \rfloor - j} b^{\lfloor \frac{t}{2} \rfloor + j} \\ &\quad - a^{\lfloor \frac{t}{2} \rfloor - j} b^{t - \lfloor \frac{t}{2} \rfloor + j} - a^{t - \lfloor \frac{t}{2} \rfloor + j} b^{\lfloor \frac{t}{2} \rfloor - j} \\ &= (a-b)^2 \beta_{t, \lfloor \frac{t}{2} \rfloor + j} + a^{\lfloor \frac{t}{2} \rfloor - j} b^{t - \lfloor \frac{t}{2} \rfloor - j} [a^{2j} - b^{2j}] \\ &\quad + a^{t - \lfloor \frac{t}{2} \rfloor - j} b^{\lfloor \frac{t}{2} \rfloor - j} [b^{2j} - a^{2j}] \\ &= (a-b)^2 \beta_{t, \lfloor \frac{t}{2} \rfloor + j} + (a^{2j} - b^{2j}) \left(a^{\lfloor \frac{t}{2} \rfloor - j} b^{t - \lfloor \frac{t}{2} \rfloor - j} - a^{t - \lfloor \frac{t}{2} \rfloor - j} b^{\lfloor \frac{t}{2} \rfloor - j} \right) \\ &= (a-b)^2 \beta_{t, \lfloor \frac{t}{2} \rfloor + j} + \frac{(a^{2j} - b^{2j}) a^{2 \lfloor \frac{t}{2} \rfloor} b^{2 \lfloor \frac{t}{2} \rfloor}}{a^{\lfloor \frac{t}{2} \rfloor + j} b^{\lfloor \frac{t}{2} \rfloor + j}} \left(b^{t-2 \lfloor \frac{t}{2} \rfloor} - a^{t-2 \lfloor \frac{t}{2} \rfloor} \right) \end{aligned}$$

but t is even, that is $t = 2r$ for some $r \in \mathbb{Z}$ and $t - 2 \lfloor \frac{t}{2} \rfloor = 0$. Therefore, $b^{t-2 \lfloor \frac{t}{2} \rfloor} - a^{t-2 \lfloor \frac{t}{2} \rfloor} = b^0 - a^0 = 0$. □

Thus, we might assume that $2 \leq s \leq \lfloor \frac{t}{2} \rfloor$ then $s - 1 < t - s$. Now, we show that if s is even in $\beta_{t,s}$ then the sequence is increasing.

Lemma 2. *The sequence $\beta_{t,2}, \beta_{t,4}, \beta_{t,6}, \dots$ that is $\{\beta_{t,2p}\}_{t,p}$ satisfies $\beta_{t,2p} < \beta_{t,2(p+1)}$ for every $p \in \{1, 2, \dots, \lfloor \frac{t}{4} \rfloor\}$ and all t .*

Proof. We have,

$$\begin{aligned}
\beta_{t,2p} &= \frac{(a^{2p} - b^{2p})(a^{t-2p} - b^{t-2p})}{(a-b)^2} \\
&= \frac{a^t - a^{2p}b^{t-2p} - a^{t-2p}b^{2p} + b^t}{(a-b)^2} \\
\beta_{t,2(p+1)} &= \frac{(a^{2p+2} - b^{2p+2})(a^{t-2p-2} - b^{t-2p-2})}{(a-b)^2} \\
\beta_{t,2p+2} &= \frac{a^t - a^{2p+2}b^{t-2p-2} - a^{t-2p-2}b^{2p+2} + b^t}{(a-b)^2} \\
(a-b)^2 \beta_{t,2p+2} &= a^t - a^{2p+2}b^{t-2p-2} - a^{t-2p-2}b^{2p+2} + b^t \\
&\quad - a^{2p}b^{t-2p} - a^{t-2p}b^{2p} \\
&\quad + a^{2p}b^{t-2p} + a^{t-2p}b^{2p} \\
&= (a-b)^2 \beta_{t,2p} + a^{2p}b^{t-2p} + a^{t-2p}b^{2p} \\
&\quad - a^{2p+2}b^{t-2p-2} - a^{t-2p-2}b^{2p+2} \\
&= (a-b)^2 \beta_{t,2p} + (1 - a^2b^{-2}) a^{2p}b^{t-2p} \\
&\quad + a^{t-2p}b^{2p}(1 - a^{-2}b^2) \\
&= (a-b)^2 \beta_{t,2p} + (b^2 - a^2) a^{2p+2}b^{t-2p} \\
&\quad + (a^2 - b^2) a^{t-2p}b^{2p+2} \\
\beta_{t,2(p+1)} &= \beta_{t,2p} + \frac{k}{(a-b)} [a^{t-2p}b^{2p+2} - a^{2p+2}b^{t-2p}] \\
&= \beta_{t,2p} + ka^{2p+2}b^{2p+2} [a^{t-4p-2} - b^{t-4p-2}] \\
&= \beta_{t,2p} + k \frac{a^{t-4p-2} - b^{t-4p-2}}{a-b} \\
&= \beta_{t,2p} + kF_{t-2(2p+1)}
\end{aligned}$$

and as $k, F_{t-2(2p+1)} > 0$, the proof is complete. \square

On the other hand, if s is odd in $\beta_{t,s}$ then the sequence is decreasing, as the following lemma shows.

Lemma 3. *The sequence $\{\beta_{t,2p+1}\}_{t,p}$ satisfies $\beta_{t,2p+1} > \beta_{t,2p+3}$ for every $p \in \{0, 2, \dots, \lfloor \frac{t}{4} \rfloor - 1\}$ and all t .*

Proof.

$$\begin{aligned}
\beta_{t,2p+1} &= \frac{(a^{2p+1} - b^{2p+1})(a^{t-2p-1} - b^{t-2p-1})}{(a-b)^2} \\
&= \frac{a^t - a^{2p+1}b^{t-2p-1} - a^{t-2p-1}b^{2p+1} + b^t}{(a-b)^2}
\end{aligned}$$

and

$$\begin{aligned}
 \beta_{t,2p+3} &= \frac{(a^{2p+3} - b^{2p+3})(a^{t-2p-3} - b^{t-2p-3})}{(a-b)^2} \\
 (a-b)^2 \beta_{t,2p+3} &= a^t - a^{2p+3}b^{t-2p-3} - a^{t-2p-3}b^{2p+3} + b^t \\
 &\quad - a^{2p+1}b^{t-2p-1} - a^{t-2p-1}b^{2p+1} \\
 &\quad + a^{2p+1}b^{t-2p-1} + a^{t-2p-1}b^{2p+1} \\
 &= (a-b)^2 \beta_{t,2p+1} + a^{2p+1}b^{t-2p-1} + a^{t-2p-1}b^{2p+1} \\
 &\quad - a^{2p+3}b^{t-2p-3} - a^{t-2p-3}b^{2p+3} \\
 &= (a-b)^2 \beta_{t,2p+1} + a^{2p+1}b^{t-2p-1} + a^{t-2p-1}b^{2p+1} \\
 &\quad - a^{2p+1}b^{t-2p-1}a^2b^{-2} - a^{t-2p-1}b^{2p+1}a^{-2}b^2 \\
 &= (a-b)^2 \beta_{t,2p+1} + a^{2p+1}b^{t-2p-1}(1 - a^2b^{-2}) \\
 &\quad + a^{t-2p-1}b^{2p+1}(1 - a^{-2}b^2)
 \end{aligned}$$

Using the fact that $ab = -1$ then $a^2b^2 = 1$, and

$$\begin{aligned}
 \beta_{t,2p+3} &= \beta_{t,2p+1} + \frac{(a^2 - b^2)a^{t-2p-1}b^{2p+3} - (a^2 - b^2)a^{2p+3}b^{t-2p-1}}{(a-b)^2} \\
 &= \beta_{t,2p+1} + k \frac{a^{t-2p-1}b^{2p+3} - a^{2p+3}b^{t-2p-1}}{a-b} \\
 &= \beta_{t,2p+1} + k(ab)^{2p+3} \frac{a^{t-4(p+1)} - b^{t-a(p+1)}}{a-b} \\
 &= \beta_{t,2p+1} - kF_{k-t-4(p+1)}
 \end{aligned}$$

and as $k, F_{k-t-4(p+1)} > 0$, the proof is complete. \square

The main Theorem of the section is the following:

Theorem 1. For any integers $t, s, k \geq 1$,

1. $\min_s \{F_s F_{t-s}\} = F_2 F_{t-2} = F_{t-2}$
2. $\max_s \{F_s F_{t-s}\} = F_1 F_{t-1} = F_{t-1}$

Proof. It is enough to proof that $\beta_{t, \lfloor \frac{t}{2} \rfloor} < \beta_{t, \lfloor \frac{t}{2} \rfloor - 1}$ which can be easily done by an algebraic manipulation and the rest of the proof follows from above lemmas. \square

4 Extremal Topologies on Polygonal Graphs

In this section, we show how the previous results about the product of Fibonacci numbers can be used for determining the structure of polygonal arrays G such that when adding a new polygon, maximize or minimize $i(G)$.

Let h be a polygon with n sides. Let P_i and P_j be two different linear paths of sizes i and j , respectively, such that $i + j = k$ becomes a constant. Let G be the resulting graph formed by joining P_i and P_j to the end-nodes of any edge $e = \{x, y\} \in E(h)$, as it is illustrated in Fig. 2. Notice that e can be any edge of the polygon since in fact, the initial polygon is a cycle and all of its edges are indistinguishable.

We show that $i(G)$ is maximum under the restriction $|P_i| + |P_j| = k$ when $i = 2$ (P_i has exactly two vertex and only one edge) and $j = k - 2$ (a path of $k - 2$ vertices).



Fig. 2. A base graph

Lemma 4. *Let h be a polygon of n sides and $e = \{x, y\} \in E(h)$. Let $P_i = \{x, x_1, \dots, x_{i-1}\}$ and $P_j = \{y, y_1, \dots, y_{j-1}\}$ be two disjoint paths such that $V(P_i) \cap V(h) = \{x\}$, $V(P_j) \cap V(h) = \{y\}$ and $i + j = k$. If $G = h \cup P_i \cup P_j$ then the maximum for $i(G)$ is achieved when $i = 2$ and $j = k - 2$.*

Proof. Applying the division edge rule on the edge $e = \{x, y\}$, we obtain that $i(G) = i(G - e) - i(G - (N[x] \cup N[y]))$. Notice that $(G - e)$ is a linear path of size $n + (i - 1) + (j - 1) = n + k - 2$; therefore, $i(G - e) = F_{n+k}$. Furthermore, $i(G - e)$ is invariant with respect to the selected position of the edge $e \in E(h)$.

On the other hand, $(G - (N[x] \cup N[y]))$ is formed by three disjoint paths: P_{i-2}, P_{j-2} and the path that results from eliminating e and its two adjacent edges from h . Let us denote this last path as P_{n-4} . Then, $i(G - (N[x] \cup N[y])) = F_{n-2} \cdot F_i \cdot F_j$. In fact, the result of this product does not depend on the initial position of e in h because the three resulting paths will have same sizes independently of the position of e in h .

Then, maximizing $i(G)$ is equivalent to minimizing $F_i \cdot F_j$ since these are the unique sizes on i and j that can vary under the restriction $i + j = k$. According to Theorem 1, $F_i \cdot F_j$ has a minimum value when $F_i = F_2$ and $F_j = F_{k-2}$ which means that the resulting path P_{i-2} after removing $N[x]$ from G should be empty and the resulting path P_{j-2} after removing $N[y]$ from G should have $k - 4$ vertices. \square

Lemma 5. *Let h be a polygon of n sides and $e = \{x, y\} \in E(h)$. Let $P_i = \{x, x_1, \dots, x_{i-1}\}$ and $P_j = \{y, y_1, \dots, y_{j-1}\}$ be two disjoint paths such that $V(P_i) \cap V(h) = \{x\}$, $V(P_j) \cap V(h) = \{y\}$ and $i + j = k$. If $G = h \cup P_i \cup P_j$ then the minimum for $i(G)$ is achieved when $i = 1$ and $j = k - 1$.*

Proof. Similar to Lemma 4. \square

Furthermore, the maximum and minimum values for $i(G)$ are achieved independently of the number of edges in the polygon h . Consequently, our results are fulfilled for any polygon joined with two disjointed paths in the end-nodes of one of its edges. We show in Fig. 3 the extremal topologies for $i(G)$ for the class of graphs: $G = h \cup P_i \cup P_j$.

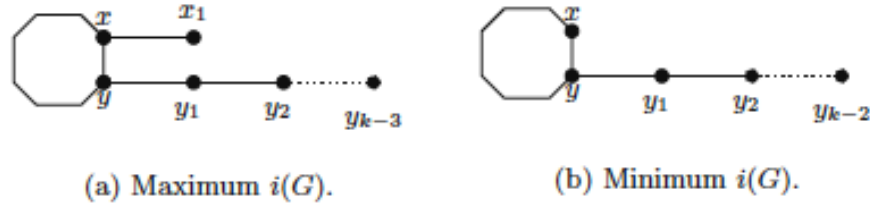


Fig. 3. Extremal topologies for $i(G)$, $G = h \cup P_i \cup P_j$.

Let $A_n : h_1, \dots, h_n, n \geq 1$ be a polygonal array and p a new polygon of k edges. We denote as e_i the common edge between the polygon h_i and h_{i+1} . We want to extend A_n to A_{n+1} joining p to A_n in such way that $i(A_{n+1})$ is either minimum or maximum into the set of possible edges $e \in E(h_n)$ to be selected for joining it with p .

Let us, enumerate the edges of h_n as b_0, b_1, \dots, b_{k-1} , where b_0 is the common edge between h_n and h_{n-1} and the numeration is according to the clockwise direction. We also consider that h_n has more than 5 edges. We must select $e \in E(h_n)$ such that $i(A_n \cup p)$ is maximum into the set of possible selections of edges of h_n . For example, e can not be anyone from b_0, b_1, b_{k-1} because if we join p to any one of those edges, then $A_n \cup p$ losses the structure of polygonal arrays.

Theorem 2. *Let A_n be a polygonal array whose last polygon h_n has k edges and p be a polygon. Let b_0, b_1, \dots, b_{k-1} be the edges of h_n such that b_0 is the common edge between h_n and h_{n-1} and the numeration is clockwise. If $A_{n+1} = A_n \cup p$ is a polygonal array then $\max\{i(A_{n+1})\}$ is achieved when p is joined to A_n at b_3 , that is a distance 2 from the common edge between h_{n-1} and h_n .*

Proof. Applying the division edge rule on $e = \{x, y\} \in E(h_n)$, we obtain

$$i(A_{n+1}) = i(A_{n+1} - e) - i(A_{n+1} - (N[x] \cup N[y])) \quad (2)$$

The term $i(A_{n+1} - e)$ is invariant from e because its values does not depend on the selected position of e to join p to A_n .

$A_{n+1} - (N[x] \cup N[y])$ is a graph formed by two connected components: a linear path P_{k-5} with $k - 5$ edges and then $i(P_{k-5}) = F_{k-2}$ that is an invariant value independent to the position of $e \in E(h_n)$. And the other connected component, denoted by G , that is a polygonal array where one of the edges in the last polygon is joined to two disjointed paths P_i and P_j . Then, $i(A_{n+1} - (N[x] \cup N[y])) = i(G) * F_{k-2}$, and that value is minimum if in G is preserved a maximum number

of edges from A_n . It means that $(N[x] \cup N[y])$ contains a minimum number of edges from p and h_n . As $\delta(x) = \delta(y) = 3$ then the minimum number of edges to be contained in $(N[x] \cup N[y])$ is 7, meaning that e has to be a distance 2 from the common edge e_{n-1} between h_{n-1} and h_n , and also $|P_i| = 0$ and $|P_j| = k - 6$, in order to maximize $i(A_{n+1})$. \square

For the minimum Merrifield-Simmon index, it is not a sufficient condition to state that p is joined to A_n to a distance one from the common edge between h_{n-1} and h_n since two cases have to be considered, Fig. 4 shows the two possible configurations in a octahedral polygonal array.

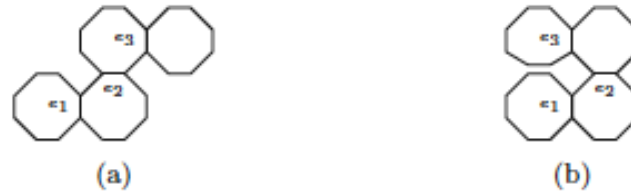


Fig. 4. In the octahedral polygonal array on the left the shortest path for visiting e_1, e_2, e_3 is a path, while it is a tree in the octahedral polygonal array on the right

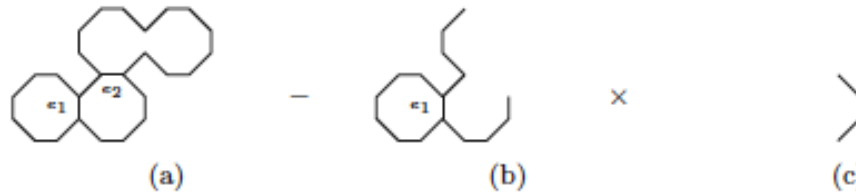


Fig. 5. Application of the edge division rule to the graph Fig. 4a to compute the Merrifield-Simmon index

Applying the edge division rule to e_3 , the decomposition to compute the Merrifield-Simmon index on the graphs Fig. 4a and b are shown in Figs. 5 and 6, respectively. The left graphs of Figs. 5a and 6a are invariant, similar to the right graphs (5c and 6c) of the same figures. By Lemma 5, the graph of Fig. 6b has minimum Merrifield-Simmon index than the graph of Fig. 5b hence the polygonal array has minimum Merrifield-Simmon index when the shortest path of e_1, e_2 and e_3 is a path.

Theorem 3. *Let A_n be a polygonal array whose last polygon h_n has k edges and p be a polygon. Let e_i be the edge joining h_i to h_{i+1} . If $A_{n+1} = A_n \cup p$ is a polygonal array then $\min\{i(A_{n+1})\}$ is achieved when p is joined to A_n at distance 1 from e_n and e_{n-1}, e_n, e_p forms a path.*

Proof. Similar to the proof of Theorem 2. \square

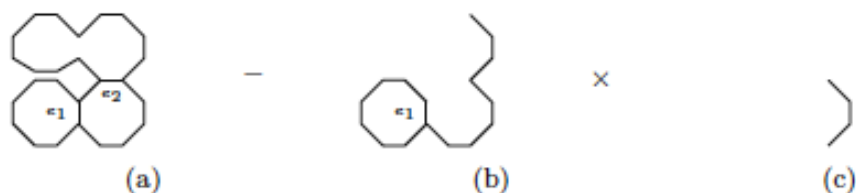


Fig. 6. Application of the edge division rule to the graph Fig. 3b to compute the Merrifield-Simmons index

5 Conclusions

We have shown how properties of Fibonacci numbers can be used for the computation of Merrifield-Simmons index. We have shown that, as expected, when adding a new polygon at distance 2, the maximum number of independent sets is obtained among all the possible combinations. Dually, the minimal number of independent sets is obtained when the distance is 1 and a path is built from the joining edges. Our method does not require to compute explicitly, the number of independent sets of the involved graphs.

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