Extremal polygonal cactus chain concerning k-independent sets *

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Abstract: In this paper we obtain the explicit recurrences of the independence polynomials of polygonal cactus chains of two classes, and show that they are the extremal polygonal cactus chains with respect to the number of independent sets.
Key words: cactus graph; h-polygonal cactus chain; k-independent set

1 Introduction

The objects nowadays known as cactus graphs appeared in the scientific literature more than half a century ago under the name of Husimi trees. Their introduction was motivated by papers of Husimi [1] and Riddell [2] dealing with cluster integrals in the theory of condensation in statistical mechanics [3]. Besides statistical mechanics, where Husimi trees and their generalizations serve as simplified models of real lattices [4, 5], the concept has also found applications in the theory of electrical and communication networks [6] and in chemistry [7, 8].

A *cactus* G is a connected graph in which each edge lies on at most a cycle. Therefore, each block in G, a maximal 2-connected subgraph of G, is either an edge or a cycle. An *h-polygon cactus* G is such a cactus that each block is an h-polygon. We call G an *h-polygon cactus chain* if each h-polygon has at most two cut vertices and each cut vertex lies on exactly two polygons. The number of h-polygons in G is called the *length* of the chains.

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Let G be an h-polygon cactus chain of length n. If $n > 1$ then G has two so called the *end h-polygons* that each one of them contains a unique cut vertex; while all the others are the *internal h-polygons*. If C is an h-polygon, then its two vertices u and v is called *j-para*-position if the distance between them is j. Specially, they are *ortho*-position if $j = 1$, and *meta*-position if $j = 2$. An internal h-polygon in G is called *ortho* if the two cut vertices that it contains are *ortho*-position. G is *ortho*-chains if its internal h-polygons are all *ortho*. *Meta*-chains can also be analogously defined.

A subset S of the vertices of a graph G is called an *independent set* of G if any two vertices of S are not adjacent, and S is called an *k-independent set* if $|S| = k$. We denote by $\alpha_k(G)$ the number of the independent sets of G with k vertices, and consider $\alpha_0(G) = 1$ and $\alpha_k(G) = 0$ if $k > \alpha(G)$, where $\alpha(G)$ is the number of the vertices of a maximum independent set of G. $i(G;x) = \sum_{k=0}^{\alpha(G)} \alpha_k(G)x^k$ is called the *independence polynomial* of G, where x is a formal variant. The number $i(G;1)$ of all independent sets of G is called the *Merrifield-Simmons index* of G in chemical terms.

In this paper we obtain the explicit recurrences of the independence polynomials of *ortho*-chains and *Meta*-chains, and show that they are the extremal polygonal cactus chains with respect to the number of independent sets.

2 Main results

Let S be a vertex of a graph G; we denote by $G - S$ the subgraph of G obtained by deleting S. In particular, if $S = \{u\}$ then we will write $G - u$ instead of $G - \{u\}$. We denote by $N[u]$ the set consisting of u and its neighborhood. In this section, we denote by O_n and M_n the *ortho*-chains and *meta*-chains of length n, respectively. The following three lemmas are due to Hosoya [9] and will be used repeatedly.

Lemma 1. *Let G be a graph and u a vertex in G. Then*

$$i(G;x) = i(G - u;x) + x \cdot i(G - N[u];x).$$

Lemma 2. *Let G be a graph consisting of the components $G_1, G_2, ..., G_k$. Then*

$$i(G;x) = i(G_1;x)i(G_2;x)\cdots i(G_k;x).$$

Lemma 3. *Suppose that P_n is a path on n vertices. Then*

$$i(P_n;x) = \sum_{k=0}^{\lfloor\frac{n+1}{2}\rfloor} \binom{n+1-k}{k} x^k.$$

We often write $i(G)$ for $i(G;x)$ unless confusion rises. For $n = 0, 1, 2$ we can verify that the independence polynomials of O_n and M_n are all equal, that is

$$\begin{aligned} i(O_0)=i(M_0) &= 1; \\ i(O_1)=i(M_1) &= i(C_h); \\ i(O_2)=i(M_2) &= i(C_h)i(P_{h-3})+xi(P_{h-1})[i(P_{h-4})+i(P_{h-3})]. \end{aligned}$$

In the following, we will use the notation G for $i(G)$, when it would lead to no confusion.

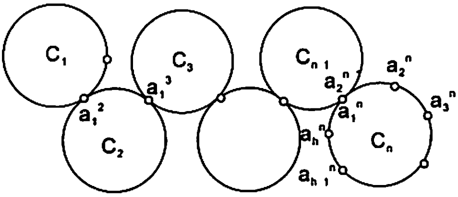

Figure 1: O_n

Theorem 4. *If $n \geq 2$, then we have*

(1) $O_n = P_{h-2}O_{n-1} + xP_{h-3}^2 O_{n-2}$;

(2) $M_n = (P_{h-3}+xP_{h-5}+xP_{h-3})M_{n-1} + (xP_{h-4}^2 - 2xP_{h-5}P_{h-3})M_{n-2}$.

Proof. Suppose that the chain O_n is as in Figure 1, where C_i is its i-th h-polygon ($1 \leq i \leq n$) and a_1^i and a_2^i are the first and second cut vertices on C_i ($2 \leq i \leq n-1$). If $n=2$ then we can easily verify that (1) is true. So we next assume $n \geq 3$. Deleting a_2^n, by Lemmas 1 and 2, we have

$$\begin{aligned} O_n &= O_n - a_2^n + x(O_n - N[a_2^n]) \\ &= P_{h-3}O_{n-1} + (xP_{h-4}+xP_{h-3})(O_{n-1} - a_2^{n-1}). \end{aligned} \quad (2.1)$$

Note that $O_{n-1} - a_2^{n-1} = O_{n-2}P_{h-3} + xP_{h-4}(O_{n-2} - a_2^{n-2})$. We have

$$O_n = P_{h-3}O_{n-1} + (xP_{h-4}+xP_{h-3})(O_{n-2}P_{h-3} + xP_{h-4}(O_{n-2} - a_2^{n-2})). \quad (2.2)$$

The result follows from (2.1) and (2.2). Similarly, we can show that (2) is also true. □

Next we will give the extremal h-polygon *cactus* chains of k-independent sets. We start with a claim; Claim 5 will be used to prove Lemma 6, from which we obtain Corollaries 7 and 8. Finally, we prove our main results by the virtue of the two Corollaries.

The following claim can be easily obtained.

Claim 5. *Let P_n be a path on n vertices. Then*

(1) $P_n = P_{n-1} + xP_{n-2}$;

(2) $P_{m+n} = P_mP_{n-1} + xP_{m-1}P_{n-2}$, $m, n \geq 0$.

Let $\mathcal{A}_n$ be a set of h-polygon cactus chains of length n. Suppose $A_n \in \mathcal{A}_n$ and denote by j the vertex labeled on the n-th h-polygon C_n of A_n, as in Figure 2. If $j \in \{2, 3, \cdots, \lfloor \frac{h}{2} \rfloor\}$ then by Lemmas 1, 2 and 3, we have

$$A_n = P_{h-3} \cdot A_{n-1} + (xP_{h-4}+xP_{h-3})(A_{n-1} - s_{n-1}), \quad (2.3)$$

$$A_n-2 = P_{h-3}\cdot A_{n-1}+xP_{h-4}(A_{n-1}-s_{n-1}), \tag{2.4}$$
$$A_n-3 = P_{h-4}\cdot A_{n-1}+(xP_{h-5}+xP_{h-3})(A_{n-1}-s_{n-1}), \tag{2.5}$$
$$A_n-j = P_{j-3}P_{h-j-1}\cdot A_{n-1}+(xP_{j-3}P_{h-j-2}+xP_{j-4}P_{h-j})(A_{n-1}-s_{n-1}). \tag{2.6}$$

Let $f(x)=\sum_{k=0}^{n} a_k x^k$ and $g(x)=\sum_{k=0}^{n} b_k x^k$ be two polynomials of x. Then we write $f(x)\preceq g(x)$ if for any k, $a_k\le b_k$ $(0\le k\le n)$; and $f(x)\prec g(x)$ if for any k, $a_k\le b_k$ and there exists some k such that $a_k<b_k$ $(0\le k\le n)$.

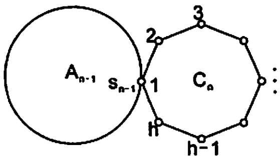

Figure 2: A_n

Lemma 6. *For $n\ge 2$, if A_n is as in Figure 2, and $j\in\{4,\cdots,\lfloor\frac{h}{2}\rfloor\}$, then $A_n-2\prec A_n-j\prec A_n-3$.*

Proof. By the above (2.4), (2.5), (2.6) and Claim 5, we have

$$\begin{aligned}&(A_n-j)-(A_n-3)\\ &=A_{n-1}(P_{j-3}P_{h-j-1}-P_{h-4})+(A_{n-1}-s_{n-1})[xP_{j-3}P_{h-j-2}\\ &\quad+xP_{j-4}P_{h-j}-xP_{h-5}-xP_{h-3}]\\ &=x^3P_{j-5}P_{h-j-3}[(A_{n-1}-N[s_{n-1}])-(A_{n-1}-s_{n-1})];\end{aligned}$$

$$\begin{aligned}&(A_n-j)-(A_n-2)\\ &=A_{n-1}(P_{j-3}P_{h-j-1}-P_{h-3})+(A_{n-1}-s_{n-1})[xP_{j-3}P_{h-j-2}\\ &\quad+xP_{j-4}P_{h-j}-xP_{h-4}]\\ &=x^2P_{j-4}P_{h-j-2}[(A_{n-1}-s_{n-1})-(A_{n-1}-N[s_{n-1}])].\end{aligned}$$

Note that $(A_{n-1}-s_{n-1})-(A_{n-1}-N[s_{n-1}])\succ 0$. We have $A_n-2\prec A_n-j\prec A_n-3$. □

Lemma 6 has two immediate corollaries.

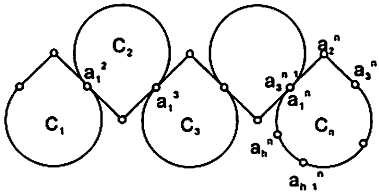

Figure 3: M_n

Corollary 7. *Suppose that O_n is as in Figure 1. Then $O_n-a_2^n\prec O_n-j\prec O_n-a_3^n$, $j\in\{4,5,\cdots,\lfloor\frac{h}{2}\rfloor\}$.*

Corollary 8. *Suppose that M_n is as in Figure 3. Then $M_n-a_2^n\prec M_n-j\prec M_n-a_3^n$, $j\in\{4,5,\cdots,\lfloor\frac{h}{2}\rfloor\}$.*

Now we can prove the following theorem which contains the results that we want.

Theorem 9. *If $A_n\in\mathcal{A}_n$ $(n\ge 3)$, then we have*

(i) $O_n - a_2^n \preceq A_n - j \preceq M_n - a_3^n \; j \in \{2,3,\cdots,\lfloor \frac{h}{2} \rfloor\}$;

(ii) $O_n \preceq A_n \preceq M_n$.

Proof. Note first that if $A_n = M_n$ or $A_n = O_n$ then the equalities in (i) and (ii) hold by Corollaries 7 and 8. Hence we assume below that $A_n \neq O_n$ and $A_n \neq M_n$. We use the induction on n. Suppose $n = 3$. Then we have

$$\begin{aligned} A_3 - j &= P_{j-3}P_{h-j-1} \cdot A_2 + (xP_{j-3}P_{h-j-2} + xP_{j-4}P_{h-j})(A_2 - s_2); \\ M_3 - a_3^3 &= P_{h-4}M_2 + (xP_{h-5} + xP_{h-3})(M_2 - a_3^2); \end{aligned}$$

$$\begin{aligned} A_3 - j &= P_{j-3}P_{h-j-1} \cdot A_2 + (xP_{j-3}P_{h-j-2} + xP_{j-4}P_{h-j})(A_2 - s_2); \\ O_3 - a_2^3 &= P_{h-3}O_2 + xP_{h-4}(O_2 - a_2^2). \end{aligned}$$

Thus by Corollaries 7 and 8, we know

$$\begin{aligned} &(A_3 - j) - (M_3 - a_3^3) \\ &= (P_{j-1}P_{h-j-1} - P_{h-4})M_2 + (xP_{j-3}P_{h-j-2} + xP_{j-4}P_{h-j})(M_2 - s_2) \\ &\quad - (xP_{h-5} + xP_{h-3})(M_2 - a_3^2) \\ &\prec (P_{j-2}P_{h-j} - P_{h-3})M_2 + (xP_{j-3}P_{h-j-2} + xP_{j-4}P_{h-j} \\ &\quad - xP_{h-5} - xP_{h-3})(M_2 - a_3^2) \\ &= x^3P_{j-5}P_{h-j-3}[(M_2 - N[a_3^2]) - (M_2 - a_3^2)] \prec 0; \end{aligned}$$

$$\begin{aligned} &(A_3 - j) - (O_3 - a_2^3) \\ &= P_{j-3}P_{h-j-1} \cdot A_2 + (xP_{j-3}P_{h-j-2} + xP_{j-4}P_{h-j})(A_2 - s_2) - P_{h-3}O_2 \\ &\quad - xP_{h-4}(O_2 - a_2^2) \\ &\succ (P_{j-3}P_{h-j-1} - P_{h-3})O_2 + (xP_{j-3}P_{h-j-2} + xP_{j-4}P_{h-j} \\ &\quad - xP_{h-4})(O_2 - a_2^2) \\ &= x^2P_{j-4}P_{h-j-2}[(O_2 - a_2^2) - (O_2 - N[a_2^2])] \succ 0. \end{aligned}$$

We also note

$$\begin{aligned} A_3 &= P_{h-3}A_2 + (xP_{h-4} + xP_{h-3})(A_2 - s_2) \\ &= P_{h-3}M_2 + (xP_{h-4} + xP_{h-3})(M_2 - s_2) \\ &\text{or } P_{h-3}O_2 + (xP_{h-4} + xP_{h-3})(O_2 - s_2); \\ M_3 &= P_{h-3}M_2 + (xP_{h-4} + xP_{h-3})(M_2 - a_3^2); \\ O_3 &= P_{h-3}O_2 + (xP_{h-4} + xP_{h-3})(O_2 - a_2^2). \end{aligned}$$

By Corollaries 7 and 8, we know that $M_2 - s_2 \prec M_2 - a_3^2$ and $O_2 - s_2 \succ O_2 - a_2^2$. Hence $A_3 \prec M_3$ and $A_3 \succ O_3$.

Next we assume $n \geq 4$. Note that any A_n of $\mathcal{A}_n$ can be obtained from an appropriately chosen graph $A_{n-1} \in \mathcal{A}_{n-1}$ by attaching to it a new h-polygon C_n, as in Figure 2. By the inductive hypothesis that $A_{n-1} - s_{n-1} \prec M_{n-1} - a_3^{n-1}$ and $A_{n-1} \prec M_{n-1}$; $A_{n-1} - s_{n-1} \succ O_{n-1} - a_2^{n-1}$ and $A_{n-1} \succ O_{n-1}$, we have

$$\begin{aligned} &(A_n - j) - (M_n - a_3^n) \\ &= P_{j-3}P_{h-j-1}A_{n-1} + (A_{n-1} - s_{n-1})(xP_{j-3}P_{h-j-2} + xP_{j-4}P_{h-j}) \\ &\quad - P_{h-4}M_{n-1} - (M_{n-1} - a_3^{n-1})(xP_{h-5} + xP_{h-3}) \\ &\prec (P_{j-3}P_{h-j-1} - P_{h-4})M_{n-1} + (M_{n-1} - a_3^{n-1})(xP_{j-3}P_{h-j-2} \\ &\quad + xP_{j-4}P_{h-j} - xP_{h-5} - xP_{h-3}) \\ &= x^3P_{j-5}P_{h-j-3}[(M_{n-1} - N[a_3^{n-1}]) - (M_{n-1} - a_3^{n-1})] \prec 0; \end{aligned}$$

$$
\begin{aligned}
&(A_n - j) - (O_n - a_2^n) \\
&= P_{j-3}P_{h-j-1}A_{n-1} + (A_{n-1} - s_{n-1})(xP_{j-3}P_{h-j-2} + xP_{j-4}P_{h-j}) \\
&\quad - P_{h-3}O_{n-1} - xP_{h-4}(O_{n-1} - a_2^{n-1}) \\
&\succ (P_{j-3}P_{h-j-1} - P_{h-4})O_{n-1} + (O_{n-1} - a_2^{n-1})(xP_{j-3}P_{h-j-2} \\
&\quad + xP_{j-4}P_{h-j} - xP_{h-4}) \\
&= x^2P_{j-4}P_{h-j-2}[(O_{n-1} - a_2^{n-1}) - (O_{n-1} - N[a_2^{n-1}])] \succ 0.
\end{aligned}
$$

Thus (i) is finished.

By (2.3) we know

$$
\begin{aligned}
A_n &= P_{h-1} \cdot A_{n-1} + 2xP_{h-2}(A_{n-1} - s_{n-1}); \\
M_n &= P_{h-1}M_{n-1} + 2xP_{h-2}(M_{n-1} - a_3^{n-1}); \\
O_n &= P_{h-1}O_{n-1} + 2xP_{h-2}(O_{n-1} - a_2^{n-1}).
\end{aligned}
$$

By (i) we know $M_{n-1} - a_3^{n-1} \succ A_{n-1} - s_{n-1}$. Therefore, by the inductive hypothesis that $M_{n-1} \succ A_{n-1}$, we have $A_n \prec M_n$. Similarly, we can also prove $A_n \succ O_n$. □

As a consequence of Theorem 9, we have

Theorem 10. *If $A_n \in \mathcal{A}_n$ then $\alpha_k(O_n) \preceq \alpha_k(A_n) \preceq \alpha_k(M_n)$. In addition, for all k, $\alpha_k(O_n) \prec \alpha_k(A_n) \prec \alpha_k(M_n)$ unless $A_n = M_n$ or $A_n = O_n$.*

The following theorem is equivalent to Theorem 10.

Theorem 11. *For $A_n \in \mathcal{A}_n$, we have*

(i) *If $A_n \neq O_n$, then $i(A_n, 1) \succ i(O_n, 1)$,*

(ii) *If $A_n \neq M_n$ then $i(A_n, 1) \prec i(M_n, 1)$.*

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