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INDEPENDENCE POLYNOMIALS OF SOME GRAPHS WITH EXTREMAL FIBONACCI INDEX

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Abstract. An *independent* set in a graph G is a set of pairwise non-adjacent vertices, and the *independence number* $\alpha(G)$ is the cardinality of a maximum stable set in G. The *independence polynomial* of G is

$$I(G;x) = s_0 + s_1x + s_2x^2 + ... + s_\alpha x^\alpha, \alpha = \alpha(G),$$

where s_k is the number of independent sets of size k in G (I. Gutman and F. Harary, 1983). The *Fibonacci index* $Fib(G)$ of a graph G is the number of all its independent set, i.e., $Fib(G) = I(G;1)$. Tight lower and upper bounds for Fibonacci index are known for general graphs, connected or not, and the corresponding extremal graphs are characterized [6], [15].

In this paper, we give explicit formulae for independence polynomials of these extremal graphs, which we further use to analyze some of their properties (unimodality, log-concavity).

1. INTRODUCTION

Throughout this paper $G = (V, E)$ is a finite, undirected, loopless and without multiple edges graph, whose vertex set is $V = V(G)$ and edge set is $E = E(G)$. $G[X]$ is the subgraph of G induced by $X \subset V$, while $G - X$ means the subgraph $G[V - X]$.

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We also denote by $G-F$ the partial subgraph of G obtained by deleting the edges of F, for $F \subset E(G)$, and we write shortly $G-e$, whenever $F=\{e\}$. The *neighborhood* of $v \in V$ is the set $N_G(v) = \{w : w \in V \text{ and } vw \in E\}$, and $N_G[v] = N_G(v) \cup \{v\}$; if there is no ambiguity on G, we use $N(v)$ and $N[v]$, respectively.

The *disjoint union* of the graphs G_1, G_2 is the graph $G = G_1 \cup G_2$ having $V(G)$ and $E(G)$ equal to the disjoint union of $V(G_1), V(G_2)$, and the disjoint union of $E(G_1), E(G_2)$, respectively. In particular, nG equals the disjoint union of $n \geq 2$ copies of the graph G. The *Zykov sum* of two disjoint graphs G_1, G_2 is the graph denoted by G_1+G_2 and having $V(G) = V(G_1) \cup V(G_2)$ as a vertex set and $E(G_1) \cup E(G_2) \cup \{v_1v_2 : v_1 \in V(G_1), v_2 \in V(G_2)\}$ as an edge set.

By an *independent* (or *stable*) set in G we mean a set of pairwise non-adjacent vertices. A stable set of maximum size will be referred to as a *maximum stable set* of G, and $\alpha(G)$ is the size of a maximum stable set in G.

If s_k equals the number of stable sets of size k in a graph G, then the polynomial

$$I(G;x) = s_0 + s_1x + s_2x^2 + ... + s_\alpha x^\alpha, \alpha = \alpha(G),$$

is called the *independence polynomial* of G, (Gutman and Harary, [8]), or the *independent set polynomial* of G (Hoede and Li, [10]). The reader is referred to [12] for a survey on these graph polynomials.

Proposition 1.1. [8] *The following equalities are true:*
(i) $I(G_1 \cup G_2; x) = I(G_1; x) \cdot I(G_2; x)$;
(ii) $I(G_1 + G_2; x) = I(G_1; x) + I(G_2; x) - 1$;
(iii) $I(G; x) = I(G-v; x) + x \bullet I(G-N[v]; x)$ *holds for each* $v \in V(G)$.

A polynomial $a_0+a_1x+a_2x^2+...+a_nx^n$, whose coefficients are real, is called:

- *unimodal* if there is some $k \in \{0,1,...,n\}$, called *mode*, such that
$$a_0 \leq ... \leq a_{k-1} \leq a_k \geq a_{k+1} \geq ... \geq a_n;$$
- *log-concave* if $a_i^2 \geq a_{i-1} \cdot a_{i+1}, i \in \{1,2,...,n-1\}$.

For instance, the independence polynomial

- $I(K_{42} + 3K_7; x) = 1 + 63x + 147x^2 + 343x^3$ is log-concave and has only one real root;
- $I(K_{43} + 3K_7; x) = 1 + 64x + 147x^2 + 343x^3$ is unimodal, but non-log-concave, because $147^2 - 64 \cdot 343 = -343 < 0$;

- $I(K_{127} + 3K_7; x) = 1 + 148x + 147x^2 + 343x^3$ is non-unimodal.

The unimodality of independence polynomials was studied in a number of papers, like [1], [2], [9], [13], [18].

It is known that each log-concave polynomial of positive coefficients is also unimodal.

Theorem 1.2. *(Newton Inequality) If $P = a_0 + a_1x + ... + a_nx^n$ is a polynomial with nonnegative coefficients, and all its roots are real, then*

$$(a_k)^2 \geq a_{k-1} \bullet a_{k+1} \bullet \frac{k+1}{k} \bullet \frac{n-k+1}{n-k}, 1 \leq k \leq n-1.$$

Hence P is log-concave and unimodal with at most two modes.

The independence polynomial can have non-real roots and this is true also for trees, e.g., $I(K_{1,3}; x) = 1 + 4x + 3x^2 + x^3$. Brown *et al.* showed that the independence polynomial of every graph has at least one real root.

Theorem 1.3. [4] *For any graph G, a root of the independence polynomial of G of smallest modulus is real.*

The product of two polynomials, one log-concave and the other unimodal, is not always log-concave, for instance, if $G = K_{40} + 3K_7$ and $H = K_{110} + 3K_7$, then

$$\begin{aligned} &I(G; x) \cdot I(H; x) = \\ &= (1 + 61x + 147x^2 + 343x^3)(1 + 131x + 147x^2 + 343x^3) \\ &= 1 + 192x + 8285x^2 + 28910x^3 + 87465x^4 + 100842x^5 + 117649x^6, \end{aligned}$$

which is not log-concave, because $100842^2 - 87465 \cdot 117649 < 0$. However, the following result, due to Keilson and Gerber, gives a sufficient condition for two polynomials to have a unimodal product.

Theorem 1.4. [11] *If P is log-concave and Q is unimodal, then $P \cdot Q$ is unimodal, while the product of two log-concave polynomials is log-concave.*

The *corona* of the graphs G and H is the graph $G \circ H$ obtained from G and $|V(G)|$ copies of H, such that each vertex of G is joined to all vertices of a copy of H. The connection between the independence polynomials of G, H and $G \circ H$ is given by the following result, due to I. Gutman.

Theorem 1.5. [9] $I(G \circ H; x) = (I(H; x))^n \cdot I(G; \frac{x}{I(H;x)})$, *where n is the order of G.*

For example, if $G = \overline{K_n}$, then $\alpha(G) = n$ and $G \circ K_p = nK_{p+1}$ has $I(G \circ K_p; x) = (1 + (p+1) \cdot x)^n$, whose roots are all real.

The *Fibonacci index* of a graph G is the number of all its independent sets [16]. In other words, the Fibonacci index of G is equal to $I(G; 1) = s_0 + s_1 + s_2 + ... + s_\alpha$. This parameter was defined independently by Merrifield and Simmons [14] in the chemistry literature, where it has been extensively studied, especially in chemical graph theory.

For instance, we have:

- $I(K_n; x) = 1 + nx$, hence $Fib(K_n) = n + 1$;
- $I(\overline{K_n}; x) = (1 + x)^n$, hence $Fib(\overline{K_n}) = 2^n$;
- $I(P_n; x) = \sum\limits_{k=0}^{\lceil n/2 \rceil} \binom{n+1-k}{k} \cdot x^k$, and $Fib(P_n) = f_{n+2}$ (recall that the sequence of Fibonacci numbers f_n is $f_0 = 0, f_1 = 1$ and $f_n = f_{n-1} + f_{n-2}$ for $n > 1$).

In this paper we give explicit formulae for independence polynomials of graphs whose Fibonacci index is extremal.

2. RESULTS

In extremal graph theory, lower and upper bounds for $Fib(G)$ inside the classes of general graphs, connected graphs, and trees are well known. The lower bound for the Fibonacci index is known for general graphs.

Let us denote $CS_{n,\alpha} = \alpha K_1 + K_{n-\alpha}$, for $1 \le \alpha \le n - 1$. Clearly, $\alpha(CS_{n,\alpha}) = \alpha$.

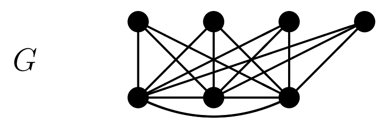

FIGURE 1. $G = CS_{7,4}$.

Pedersen and Vestergaard characterize graphs with minimum Fibonacci index as follows.

Theorem 2.1. [15] *If G is a graph of order n and $\alpha(G) = \alpha$, then $Fib(G) \ge 2^\alpha + n - \alpha$, with equality if and only if G is isomorphic to $CS_{n,\alpha}$.*

Using Proposition 1.1*(ii)* we deduce the following.

Theorem 2.2. *The independence polynomial of $CS_{n,\alpha}$ satisfies:*
(i) $I\left(CS_{n,\alpha};x\right) = (1+x)^{\alpha} + (n-\alpha)\,x$,
hence $Fib(CS_{n,\alpha}) = 2^{\alpha} + n - \alpha$;
(ii) $I\left(CS_{n,\alpha};x\right)$ *is unimodal for*
(1) $1 \leq \alpha \leq 6$ *and* $\alpha < n$, *or* (2) $6 < \alpha < n < \binom{\alpha}{2}$;
(iii) $I\left(CS_{n,\alpha};x\right)$ *is log-concave for*
(1) $\alpha \in \{1,2\}$ *and* $3 \leq n$, *or* (2) $3 \leq \alpha < n \leq \frac{3\alpha(\alpha-1)}{2(\alpha-2)}$.

Proof. *(i)* Since, in fact, we have $CS_{n,\alpha} = \alpha K_1 + K_{n-\alpha}$, Proposition 1.1*(ii)* implies

$$I\left(CS_{n,\alpha};x\right) = I\left(\alpha K_1;x\right) + I\left(K_{n-\alpha};x\right) - 1 = (1+x)^{\alpha} + (n-\alpha)\,x =$$
$$= 1 + nx + \binom{\alpha}{2}x^2 + \binom{\alpha}{3}x^3 + ... + \ x^{\alpha},$$

which clearly implies $Fib(CS_{n,\alpha}) = I\left(CS_{n,\alpha};1\right) = 2^{\alpha} + n - \alpha$.

(ii) and *(iii)* Clearly, for $\alpha \in \{1,2\} \Rightarrow I\left(CS_{n,\alpha};x\right)$ has only real roots, hence $I\left(CS_{n,\alpha};x\right)$ is unimodal and log-concave.

- *Case* $\alpha = 3$. Then $I\left(CS_{n,3};x\right) = 1 + nx + 3x^2 + x^3$, which is

(a) unimodal for $n \geq \alpha + 1 = 4$; *(b)* log-concave for $4 \leq n \leq 9$.

- *Case* $\alpha = 4$. Then $I\left(CS_{n,4};x\right) = 1 + nx + 6x^2 + 4x^3 + x^4$ and this is

(a) unimodal for $n \geq \alpha + 1 = 5$; *(b)* log-concave for $5 \leq n \leq 9$.

- *Case* $\alpha = 5$. Then $I\left(CS_{n,5};x\right) = 1+nx+10x^2+10x^3+5x^4+x^5$, which is

(a) unimodal for $n \geq \alpha + 1 = 6$; *(b)* log-concave for $6 \leq n \leq 10$.

- *Case* $\alpha = 6$. Then $I\left(CS_{n,6};x\right) = 1+nx+15x^2+20x^3+15x^4+6x^5+x^6$, which is

(a) unimodal for $n \geq \alpha + 1 = 7$ and $n \leq 15 = \binom{6}{2}$, i.e., $7 \leq n \leq 15$; *(b)* log-concave for $7 \leq n \leq 11$.

In general, for $\alpha > 6$, it follows that:

- $I\left(CS_{n,\alpha};x\right)$ is unimodal for $\alpha + 1 \leq n \leq \binom{\alpha}{2}$;
- $I\left(CS_{n,\alpha};x\right)$ is log-concave whenever

$$7 < \alpha + 1 \leq n, n^2 \geq \binom{\alpha}{2}, \binom{\alpha}{2} \bullet \binom{\alpha}{2} \geq n \bullet \binom{\alpha}{3},$$

which lead to $7 < \alpha + 1 \leq n \leq \frac{3\alpha(\alpha-1)}{2(\alpha-2)}$.

□

For instance, the polynomial

- $I\left(CS_{10,7};x\right)=\left(1+x\right)^{7}+3x=1+10x+21x^{2}+35x^{3}+35x^{4}+21x^{5}+7x^{6}+x^{7}$ is log-concave;
- $I(CS_{12,6};x)=1+12x+15x^{2}+20x^{3}+15x^{4}+6x^{5}+x^{6}$ is unimodal, but is not log-concave, because $15^{2}-12\cdot 20=225-240=-15<0$;
- $I(CS_{22,6};x)=1+22x+21x^{2}+35x^{3}+35x^{4}+21x^{5}+7x^{6}+x^{7}$ is not unimodal.

The *Turán graph* $T(n,k)$ is a graph formed by partitioning a set of n vertices into k subsets, with sizes as equal as possible, and connecting two vertices by an edge whenever they belong to different subsets. The graph $T(n,k)$ will have $q=n \bmod k$ subsets of size $\lceil n/k\rceil$, and $k-q$ subsets of size $\lfloor n/k\rfloor$. In other words, $T(n,k)$ is a complete k-partite graph, i.e., $T(n,k)=K_{\lceil n/k\rceil,\lceil n/k\rceil,\ldots,\lfloor n/k\rfloor,\lfloor n/k\rfloor}$, and clearly, $\alpha\left(T(n,k)\right)=\lceil n/k\rceil$. According to Turán's Theorem, the Turán graph has the maximum possible number of edges among all $(k+1)$-clique-free graphs.

Theorem 2.3. *The independence polynomial of the Turán graph $T(n,k)$ satisfies:*

(i) $I\left(T(n,k);x\right)=(n \bmod k)\bullet(1+x)^{\lceil n/k\rceil}+(k-(n \bmod k))\bullet(1+x)^{\lfloor n/k\rfloor}-(k-1)$, *hence*

$$Fib(T(n,k))=(n \bmod k)\bullet 2^{\lceil n/k\rceil}+(k-(n \bmod k))\bullet 2^{\lfloor n/k\rfloor}-(k-1);$$

(ii) $I\left(T(n,k);x\right)$ *is log-concave, hence unimodal, for every positive integers n and $k\leq n$;*

(iii) *if $k\geq n/2$, then $I\left(T(n,k);x\right)$ has only real roots.*

Proof. *(i)* Using Proposition 1.1*(ii)*, we get that

$$\begin{aligned} I\left(T(n,k);x\right)=I\left(K_{\lceil n/k\rceil,\lceil n/k\rceil,\ldots,\lfloor n/k\rfloor,\lfloor n/k\rfloor};x\right)= \\ =(n \bmod k)\bullet(1+x)^{\lceil n/k\rceil}+ \\ +(k-(n \bmod k))\bullet(1+x)^{\lfloor n/k\rfloor}-(k-1), \end{aligned}$$

which implies

$$Fib(T(n,k))=(n \bmod k)\bullet 2^{\lceil n/k\rceil}+(k-(n \bmod k))\bullet 2^{\lfloor n/k\rfloor}-(k-1).$$

(ii) Since the polynomials

$$P_1=(n \bmod k)\bullet(1+x)^{\lceil n/k\rceil} \text{ and } P_2=(k-(n \bmod k))\bullet(1+x)^{\lfloor n/k\rfloor}$$

satisfy $0\leq\deg\left(P_1\right)-\deg\left(P_2\right)\leq 1$, it is easy to see that $P=P_1+P_2$ has only real roots, and because P has only positive coefficients, it follows that P is log-concave by Newton's Theorem 1.2. Consequently, $I(T(n,k);x) = P - (k-1)$ is log-concave, and unimodal as well, because its free coefficient is equal to 1.

(iii) If $k \geq n/2$, then $I(T(n,k);x)$ is a polynomial of degree at most two, since $\alpha(I(T(n,k);x)) \leq 2$. Consequently, by Theorem 1.3, $I(T(n,k);x)$ has real roots. $\square$

Remark 2.4. *Notice that $I(T(n,k);x)$ may have only real roots for $k < n/2$; e.g., $I(T(9,4);x) = (1+x)^3 + 3(1+x)^2 - 3 = 0$, has only real roots. However, $I(T(8,3);x) = 2(1+x)^3 + (1+x)^2 - 2$ has only one real root.*

Clearly, the complement of the Turán graph $T(n,\alpha)$, that we denote by $TC(n,\alpha) = \overline{T(n,\alpha)}$, is the disjoint union of α balanced cliques, and $\alpha(TC(n,\alpha)) = \alpha$.

Theorem 2.5. [6] *Let G be a graph of order n with independence number α. Then $Fib(G) \leq Fib(TC(n,\alpha))$, with equality if and only if G is isomorphic to $TC(n,\alpha)$.*

Theorem 2.6. *The independence polynomial of the complement of Turán graph $TC(n,\alpha)$ satisfies:*

(i) $I(TC(n,\alpha);x) =$
$= (1 + \lceil n/\alpha \rceil \bullet x)^{(n \bmod \alpha)} \bullet (1 + \lfloor n/\alpha \rfloor \bullet x)^{\alpha-(n \bmod \alpha)}$;

(ii) *$I(TC(n,\alpha);x)$ has only real roots for every n and $\alpha \leq n$; hence $I(TC(n,\alpha);x)$ is always log-concave and unimodal.*

Proof. (i) Using Proposition 1.1*(i)*, we get that

$$\begin{aligned} I(TC(n,\alpha);x) &= I\left(\overline{K_{\lceil n/\alpha \rceil, \lceil n/\alpha \rceil, \ldots, \lfloor n/\alpha \rfloor, \lfloor n/\alpha \rfloor}}, x\right) = \\ &= \left[I\left(K_{\lceil n/\alpha \rceil}; x\right)\right]^{(n \bmod \alpha)} \bullet \left[I\left(K_{\lfloor n/\alpha \rfloor}; x\right)\right]^{\alpha-(n \bmod \alpha)} \\ &= (1 + \lceil n/\alpha \rceil \bullet x)^{(n \bmod \alpha)} \bullet (1 + \lfloor n/\alpha \rfloor \bullet x)^{\alpha-(n \bmod \alpha)}, \end{aligned}$$

as claimed.

(ii) Clearly, $I(TC(n,\alpha);x)$ has all its roots real. Newton's Theorem 1.2 implies that $I(TC(n,\alpha);x)$ is also log-concave and unimodal. $\square$

Theorem 2.6*(i)* immediately implies the following.

Corollary 2.7. [6] *The Fibonacci index of the complement of the Turán graph $TC(n,\alpha)$ is given by the formula*

$$Fib(TC(n,\alpha)) = (1 + \lceil n/\alpha \rceil)^{(n \bmod \alpha)} \bullet (1 + \lfloor n/\alpha \rfloor)^{\alpha-(n \bmod \alpha)}.$$

The *connected complement of Turán graph* with n vertices and independence number α where $1 \leq \alpha \leq n-1$, denoted by $TCC(n, \alpha)$, is constructed from $TC(n,\alpha)$ with $\alpha - 1$ additional edges, as follows: take a vertex v of one clique of size $\lceil n/\alpha \rceil$, and link v, by an edge, to one vertex belonging to each of the remaining cliques. See Figure 2 for an example.

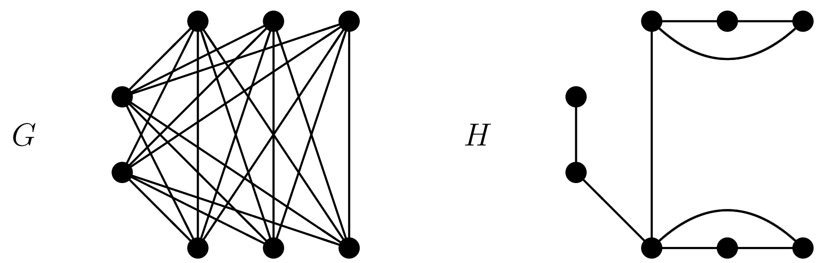

FIGURE 2. $G = T(8,3)$ and its connected complement $H = TCC(8,3)$.

Theorem 2.8. [6] *If G is a connected graph of order n with independence number α, then $Fib\,(G) \leq Fib(TCC(n,\alpha))$, with equality if and only if G is isomorphic to $TCC(n,\alpha)$ in case of $(n,\alpha) \neq (5,2)$, and G is isomorphic either to $TCC(5,2)$ or to C_5 in case of $(n,\alpha) = (5,2)$.*

Proposition 2.9. *The independence polynomial of the connected complement of Turán graph $TCC(n,\alpha)$ satisfies:*

(i) *if $n = t\alpha$, for some integer $t \geq 2$, then*

$$I\,(TCC(n,\alpha);x) = (1+(t-1)\,x) \bullet (1+tx)^{\alpha-1} + x\,(1+(t-1)\,x)^{\alpha-1},$$

$$\textit{and } Fib\,(TCC(n,\alpha)) = t \bullet (1+t)^{\alpha-1} + t^{\alpha-1};$$

(ii) *otherwise*

$$I\,(TCC(n,\alpha);x) = (1+(k_1-1)\,x) \bullet$$

$$\bullet \left\{ (1+k_1x)^{p-1}(1+k_2x)^q + x \cdot (1+(k_1-1)\,x)^{p-2}(1+(k_2-1)\,x)^q \right\},$$

$$\textit{and } Fib\,(TCC(n,\alpha)) = k_1 \bullet (1+k_1)^{p-1} \bullet (1+k_2)^q + k_1^{p-1} \bullet k_2^q,$$

where $k_1 = \lceil n/\alpha \rceil$, $k_2 = \lfloor n/\alpha \rfloor$, $p = n \bmod \alpha$, $q = \alpha - p$.

Proof. If $n = t\alpha$, then all the α cliques of $TC(n,\alpha)$ are of size t, and using Proposition 1.1*(iii)*, we get

$$\begin{aligned} I\,(TCC(n,\alpha);x) &= I\,(TCC(n,\alpha)-v;x) + x \bullet I\,(TCC(n,\alpha)-N[v];x) = \\ &= (1+(t-1)\,x) \bullet (1+tx)^{\alpha-1} + x \bullet (1+(t-1)\,x)^{\alpha-1}, \end{aligned}$$

which clearly gives $Fib\,(TCC(n,\alpha)) = t \bullet (1+t)^{\alpha-1} + t^{\alpha-1}$.

Otherwise, let

$$k_1 = \lceil n/\alpha \rceil, k_2 = \lfloor n/\alpha \rfloor, p = n \bmod \alpha, q = \alpha - p,$$

and let v be the vertex joined to all the cliques of $TCC(n,\alpha)$.

Taking into account that the both graphs $TCC(n,\alpha) - v$ and $TCC(n,\alpha) - N[v]$ are disjoint union of cliques, Proposition 1.1*(iii)* leads to the following

$$\begin{aligned} I\,(TCC(n,\alpha);x) &= (1+(k_1-1)\,x) \bullet (1+k_1x)^{p-1} \bullet (1+k_2x)^q + \\ &+x \bullet (1+(k_1-1)\,x)^{p-1} \bullet (1+(k_2-1)\,x)^q = \\ &= (1+(k_1-1)\,x)\,\{(1+k_1x)^{p-1}\,(1+k_2x)^q + \\ &+x \bullet (1+(k_1-1)\,x)^{p-2} \cdot (1+(k_2-1)\,x)^q\}, \end{aligned}$$

which immediately implies that

$Fib\,(TCC(n,\alpha)) = k_1 \bullet (1+k_1)^{p-1} \bullet (1+k_2)^q + k_1^{p-1} \bullet k_2^q$. □

Using Theorem 2.8, Proposition 2.9, and the fact that for every tree T it is true that $\alpha\,(T) \geq |V\,(T)|\,/2$, we infer the following.

For instance, the polynomial

- $I\,(TCC(8,4);x) = 1 + 8x + 21x^2 + 23x^3 + 9x^4$ has non-real roots;
- $I\,(TCC(9,3);x) = 1 + 9x + 25x^2 + 22x^3$ has all the roots real;
- $I\,(TCC(14,4);x) = 1 + 14x + 70x^2 + 151x^3 + 120x^4$ has non-real roots;
- $I\,(TCC(11,3);x) = 1 + 11x + 38x^2 + 42x^3$ has all the roots real.

Corollary 2.10. [6] *Let T be a tree of order n with independence number α. Then $Fib(T) \leq 3^{n-\alpha-1}2^{2\alpha-n+1} + 2^{n-\alpha-1}$, with equality if and only if T is isomorphic with $TCC\,(n,\alpha)$.*

3. Conclusions and open problems

In this paper we found the independence polynomials of several graphs, whose Fibonacci index is extremal. For some of them we proved that are unimodal, log-concave, or that they have only real roots. A couple of examples above show that the independence polynomial of the connected complement of Turán graph $TCC(n,\alpha)$ may have non-real roots, but they are still log-concave. Checking many other cases, we are led to the following.

Conjecture 3.1. *The independence polynomial of $TCC(n, \alpha)$ is log-concave, for every n and $\alpha \leq n$.*

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