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INDEPENDENCE AND PI POLYNOMIALS FOR FEW STRINGS

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Abstract. If s_k is the number of independent sets of cardinality k in a graph G, then $I(G;x) = s_0 + s_1x + \ldots + s_\alpha x^\alpha$ is the independence polynomial of G [Gutman, I. and Harary, F., Generalizations of the matching polynomial, Utilitas Mathematica 24 (1983) 97-106] , where $\alpha = \alpha(G)$ is the size of a maximum independent set. Also the PI polynomial of a molecular graph G is defined as $A + \sum x^{|E(G)|-N(e)}$, where $N(e)$ is the number of edges parallel to e, $A = |V(G)|(|V(G)| + 1)/2 - |E(G)|$ and summation goes over all edges of G. In [T. Došlić, A. Loghman and L. Badakhshian, Computing Topological Indices by Pulling a Few Strings, MATCH Commun. Math. Comput. Chem. 67 (2012) 173-190], several topological indices for all graphs consisting of at most three strings are computed. In this paper we compute the PI and independence polynomials for graphs containing one, two and three strings.
Keywords. independent sets; molecular graph; independence polynomials.

1. Introduction

Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-sets of which are represented by $V(G)$ and $E(G)$, respectively. The set of neighbors of the vertex v will be denoted by $N_G(v)$, if there is no confusion we will simply write $N(v)$ instead of $N_G(v)$. The closed neighborhood of the vertex v is $N_G[v] = N_G(v) \cup \{v\}$. The degree of the vertex v will be denoted by $d(v) = |N_G(v)|$. For $S \subset V(G)$ the graph $G - S$ denotes the subgraph of G induced by the vertices $V(G) \setminus S$. If $e \in E(G)$ then $G - e$ denotes the graph with vertex set $V(G)$ and edge set $E(G) \setminus \{e\}$.

An edge set X is called independent if there is no vertex in common between any two edges in X. Also if this set has r elements we call r-edge set to be independent. Matching polynomial of graph G is defined by the sum of $(-1)^r q(G,r)x^{n-2r}$ [10].

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In which $q(G,r)$ is the number of r-edge independent set of G. A vertex set Y is called independent if there is no edge between any two vertices in Y and if this set has r elements we call r-vertex independent set. Let s_k be the number of r-vertex independent set of cardinality k in a graph G. The polynomial

$$I(G;x)=\sum_{k=0}^{\alpha(G)} s_k x^k = s_0+s_1x+\cdots+s_{\alpha(G)}x^{\alpha(G)}$$

is called the independence polynomial of G, (Gutman and Harary,[5]). We have $s_0 = 1$, $s_1 = |V(G)|$, the number of vertices of G and $s_2 = |E(\overline{G})|$, the number of edges of the complement of G. The following results are easily obtained,(see [2] and [5, 6]). The join of two disjoint graphs G and H is the graph $G+H$ such that $V(G+H) = V(G)\cup V(H)$ and $E(G+H) = E(G)\cup E(H)\cup\{v_1v_2 : v_1 \in V(G), v_2 \in V(H)\}$.

Theorem 1.1. If G and H be two vertex-disjoint graphs. Then:

a). $I(G\cup H;x) = I(G;x)I(H;x)$

b). $I(G+H;x) = I(G;x)+I(H;x)-1$

In [2], Arocha showed that $I(P_n;x) = F_{n+1}(x)$, where $F_n(x)$, $n \geq 0$, are the so-called Fibonacci polynomials. Hoede and Li [6] obtained the following recursive formula for the independence polynomial of a graph.

Theorem 1.2. For any vertex v of a graph G, we have:

$$I(G;x) = I(G-v;x)+xI(G-N_G[v];x)$$

In [1], Ashrafi, Manoochehrian and Yousefi-Azari defined a new polynomial and they named the Padmakar-Ivan polynomial. They abbreviated this new polynomial as $PI(G,x)$, for a molecular graph G and investigate some of the elementary properties of this polynomial. PI polynomial of G is defined as follow :

$$PI(G,x)=\sum_{f\in E(G)} x^{|E(G)|-N(f)}+\frac{|V(G)|(|V(G)|+1)}{2}-|E(G)|$$

Where $N(f)$ is the number of edges parallel to f. (See survey article [8] and [11] for details)

A thread in a graph G is any maximal connected subgraph induced by a set of vertices of degree 2 in G. A string in G is a subgraph induced by a thread and the vertices adjacent to it. A graph G consists of s strings if it can be represented as a union of s strings so that any two strings have at most two vertices in common [4]. In the extreme case $s = 1$, G is either a path or a cycle, and this, together with the number of vertices, gives us complete information on G. In general, the smaller s, the more information on G is packed into its string decomposition.

The first attempt on a systematic investigation of topological indices of graphs consisting of a few strings was made in a paper by Lukovits [9]. Also in [4], Došlić and co-authors computed explicit formulas for the values of several topological indices (the eccentric connectivity index, the reverse Wiener index, the geometric-arithmetic index, two connectivity indices and two Zagreb indices) for all graphs consisting of at most three strings. The ten classes of graphs considered in paper [4] are shown in Fig 3.1.

Throughout the paper we will consider G_1 denotes a path of length k (or P_{k+1}), G_4 denotes two cycles of length k and m spliced in one vertex, and G_5 denotes three paths of lengths k, m and n spliced together in one of their respective end vertices. Further, whenever referring to the strings of the same type, we assume that the lengths increase with the lexicographic order of the corresponding notational parameter. For example, we assume $k \leq m$ in G_4, G_6 and $k \leq m \leq n$ in G_5, G_8 and G_{10}. Similarly, we take $m \leq n$ in G_7 and G_9, but do not make any assumptions about the relationship of either of them with k. Also, sometimes it will be necessary to refer to the values of the string lengths. In such cases, we put the lengths in the superscripts in the alphabetic order. For example, $G_5^{1,1,n}$ denotes a graph of type (5) whose two path-like strings have length 1. Similarly, $G_9^{1,m,n}$ denotes a graph of type (9) whose path-like string is trivial. Our notation is standard and mainly taken from [3, 7].

2. Independence and PI Polynomials for few Strings

In this section we compute independence and Pi polynomials of graphs G_i, $1 \leq i \leq 10$.

Theorem 2.1. The independence polynomial of P_n, $n \geq 3$, can be obtained from the following equality:

$$I(P_n; x) = \frac{1}{\sqrt{1+4x}}((\frac{1+\sqrt{1+4x}}{2})^{n+2} + (\frac{1-\sqrt{1+4x}}{2})^{n+2})$$

Proof. It is easy to see that $I(P_0; x) = 1$ and $I(P_1; x) = 1 + x$. By Theorem 1.2, The independence polynomial of P_n, $n \geq 3$, satisfies the following equation:

$$I(P_n; x) = I(P_{n-1}; x) + xI(P_{n-2}; x)$$

In order to solve this recurrence we use a characteristic equation. The characteristic equation corresponding to the above recurrence is:

$$\lambda^2 - \lambda - x = 0$$

This gives $\lambda = \frac{1 \pm s}{2}$, where $s = \sqrt{1+4x}$. Then we have:

$$I(P_n; x) = c_1(\frac{1+s}{2})^n + c_2(\frac{1-s}{2})^n$$

By $I(P_0;x)=1$ and $I(P_1;x)=1+x$ we can compute c_1 and c_2 are as follows:

$$\begin{aligned} c_1 &= \frac{1+2x+s}{2s}, \\ c_2 &= \frac{-1-2x+s}{2s} \end{aligned}$$

And so

$$\begin{aligned} I(P_n;x) &= (\frac{1+2x+s}{2s})(\frac{1+s}{2})^n + (\frac{-1-2x+s}{2s})(\frac{1-s}{2})^n \\ &= (\frac{1}{2^{n+1}s})((2+4x+2s)(1+s)^n - (2+4x-2s)(1-s)^n) \\ &= (\frac{1}{2^{n+1}s})((1+s)^2(1+s)^n - (1-s)^2(1-s)^n) \\ &= \frac{1}{s}[(\frac{1+s}{2})^{n+2} - (\frac{1-s}{2})^{n+2}]. \end{aligned}$$

□

We know $G_1 = P_{k+1}$ and $G_2 = C_k$ then we have:

Corollary 2.1. The independence polynomial of G_1, $k \geq 2$, is as follows:

$$I(G_1;x) = \frac{1}{s}[(\frac{1+s}{2})^{k+3} - (\frac{1-s}{2})^{k+3}]$$

Where $s = \sqrt{1+4x}$.

Corollary 2.2. The independence polynomial of G_2, $k \geq 3$, is as follows:

$$I(G_2;x) = \frac{1}{2^k}[(1+s)^k + (1-s)^k$$

Where $s = \sqrt{1+4x}$.

Proof. By Theorem 1.2, the independence polynomial of C_k satisfies the following equation:

$$I(C_k;x) = I(P_{k-1};x) + xI(P_{k-3};x)$$

and by Theorem 2.1, we have:

$$\begin{aligned} I(C_k;x) &= I(P_{k-1};x) + xI(P_{k-3};x) \\ &= \frac{1}{s}[(\frac{1+s}{2})^{k+1} - (\frac{1-s}{2})^{k+1}] + \frac{x}{s}[(\frac{1+s}{2})^{k-1} - (\frac{1-s}{2})^{k-1}] \\ &= (\frac{1}{2^{k+1}s})[((1+s)^{k+1} - (1-s)^{k+1}) + 4x((1+s)^{k-1} - (1-s)^{k-1})] \\ &= (\frac{1}{2^{k+1}s})[(1+s)^{k+1} - (1-s)^{k+1} + (s^2-1)((1+s)^{k-1} - (1-s)^{k-1})] \\ &= (\frac{1}{2^{k+1}s})[2s(1+s)^k + 2s(1-s)^k] = \frac{1}{2^k}[(1+s)^k + (1-s)^k]. \end{aligned}$$

□

Figure 3.2, shows some selected points in these graphs. Apply Theorem 1.1 and Theorem 1.2, for selected vertex u, to compute this polynomial for G_i, $3 \leq i \leq 10$.

Corollary 2.3. The independence polynomials of G_i, $3 \leq i \leq 10$, are as follows:

$$\begin{aligned}
I(G_3^{k,m};x) &= \frac{(Z^{k+2}-M^{k+2})(Z^{m+2}-M^{m+2})+x(Z^{k+1}-M^{k+1})(Z^m-M^m)}{s^2}\\
I(G_4^{k,m};x) &= \frac{(Z^{k+2}-M^{k+2})(Z^{m+2}-M^{m+2})+x(Z^{k}-M^{k})(Z^m-M^m)}{s^2}\\
I(G_5^{k,m,n};x) &= \frac{(Z^{k+2}-M^{k+2})(Z^{m+2}-M^{m+2})(Z^{n+2}-M^{n+2})}{s^3}\\
&+ \frac{x(Z^{k+1}-M^{k+1})(Z^{m+1}-M^{m+1})(Z^{n+1}-M^{n+1})}{s^3}\\
I(G_6^{k,m,n};x) &= \frac{(Z^{k+2}-M^{k+2})(Z^{m+2}-M^{m+2})(Z^{n+2}-M^{n+2})}{s^3}\\
&+ \frac{x(Z^{k+1}-M^{k+1})(Z^{m+1}-M^{m+1})(Z^{n}-M^{n})}{s^3}\\
I(G_7^{k,m,n};x) &= \frac{(Z^{n+2}-M^{n+2})(Z^{k+1}-M^{k+1})(Z^{m+2}-M^{m+2})}{s^3}\\
&+ \frac{x(Z^{n+2}-M^{n+2})(Z^{k}-M^{k})(Z^{m}-M^{m})}{s^3}\\
&+ \frac{x(Z^{n}-M^{n})(Z^{k}-M^{k})(Z^{m+2}-M^{m+2})}{s^3}\\
&+ \frac{x^2(Z^{n}-M^{n})(Z^{k-1}-M^{k-1})(Z^{m}-M^{m})}{s^3}\\
I(G_8^{k,m,n};x) &= \frac{(Z^{n+1}-M^{n+1})(Z^{k+1}-M^{k+1})(Z^{m+1}-M^{m+1})}{s^3}\\
&+ \frac{2x(Z^{n}-M^{n})(Z^{k}-M^{k})(Z^{m}-M^{m})}{s^3}\\
&+ \frac{x^2(Z^{n-1}-M^{n-1})(Z^{k-1}-M^{k-1})(Z^{m-1}-M^{m-1})}{s^3}\\
I(G_9^{k,m,n};x) &= \frac{(Z^{n+2}-M^{n+2})(Z^{k+2}-M^{k+2})(Z^{m+2}-M^{m+2})}{s^3}\\
&+ \frac{x(Z^{n}-M^{n})(Z^{k+1}-M^{k+1})(Z^{m}-M^{m})}{s^3}\\
I(G_{10}^{k,m,n};x) &= \frac{(Z^{n+2}-M^{n+2})(Z^{k+2}-M^{k+2})(Z^{m+2}-M^{m+2})}{s^3}\\
&+ \frac{x(Z^{n}-M^{n})(Z^{k}-M^{k})(Z^{m}-M^{m})}{s^3}
\end{aligned}$$

Where $s = \sqrt{1+4x}$, $Z = \frac{1+s}{2}$ *and* $M = \frac{1-s}{2}$.

Now, we are ready to compute the PI polynomial of graphs G_i, $1 \leq i \leq 10$. For computing the PI polynomial of G_i, it is enough to calculate $N(e)$, for every $e \in$

$E(G_i)$. To calculate $N(e)$, we consider two cases that e is edge of paths or edge of cycles. We start by quoting known results for paths and cycles.

Lemma 2.1. Let $G_2 = C_k$ and $G_1 = P_{k+1}$ be a cycle and a path of length k. Then we have:

$$\begin{aligned} PI(G_1,x) &= k(x^{k-1}-1)+C(k+2,2), \\ PI(G_2,x) &= \begin{cases} kx^{k-2}+C(k,2) & k \textit{ is even} \\ kx^{k-1}+C(k,2) & k \textit{ is odd} \end{cases}. \end{aligned}$$

The results for two-parameter graphs depend on the parity of the cycle length(s).

Theorem 2.2. The PI polynomial of G_3 and G_4 are computed as follows:

$$\begin{aligned} PI(G_3,x) &= \begin{cases} kx^{k+m-1}+mx^{k+m-2}+C(k+m,2) & m \textit{ is even} \\ (k+m-1)x^{k+m-1}+x^{m-1}+C(k+m,2) & m \textit{ is odd} \end{cases}, \\ PI(G_4,x) &= \begin{cases} (k+m)x^{k+m-2}+T & k,m \textit{ are even} \\ mx^{k+m-2}+(k-1)x^{k+m-1}+x^{k-1}+T & k \textit{ is odd}, m \textit{ is even} \\ kx^{k+m-2}+(m-1)x^{k+m-1}+x^{m-1}+T & m \textit{ is odd}, k \textit{ is even} \\ (k+m-2)x^{k+m-1}+x^{m-1}+x^{k-1}+T & k,m \textit{ are odd} \end{cases}. \end{aligned}$$

Where $T = \frac{(k+m)(k+m-1)}{2}$.

Proof. Consider G_3 to compute its PI polynomial. It is clear that $|E(G_3)| = |V(G_3)| = k+m$. From Figures 3.1, one can see that there are two types of edges of G_3. If $e \in E(P_{k+1})$ then $N(e) = 1$ and if $e \in E(C_m)$ then $N(e) = 1$ or 2 (m is odd or even). Now, by according to definition PI polynomial we have:

$$\begin{aligned} PI(G_3,x) &= \sum_{f\in E(G_3)} x^{|E(G_3)|-N(f)} + \frac{|V(G_3)|(|V(G_3)|+1)}{2} - |E(G_3)| \\ &= \sum_{f\in E(P_{k+1})} x^{|E(G_3)|-N(f)} + \sum_{f\in E(C_m)} x^{|E(G_3)|-N(f)} + C(k+m,2) \\ &= kx^{k+m-1} + \begin{cases} mx^{k+m-2}+C(k+m,2) & m \textit{ is even} \\ (m-1)x^{k+m-1}+x^{m-1}+C(k+m,2) & m \textit{ is odd} \end{cases} \\ &= \begin{cases} kx^{k+m-1}+mx^{k+m-2}+C(k+m,2) & m \textit{ is even} \\ (k+m-1)x^{k+m-1}+x^{m-1}+C(k+m,2) & m \textit{ is odd} \end{cases}. \end{aligned}$$

To compute $PI(G_4,x)$, we consider four separate cases as follow:

$$\begin{aligned} PI(G_4,x) &= \sum_{f\in E(G_4)} x^{|E(G_4)|-N(f)} + \frac{|V(G_4)|(|V(G_4)|+1)}{2} - |E(G_4)| \\ &= \sum_{f\in E(C_k)} x^{|E(G_3)|-N(f)} + \sum_{f\in E(C_m)} x^{|E(G_3)|-N(f)} + \frac{(k+m)(k+m-1)}{2} \end{aligned}$$

$$= \begin{cases} (k+m)x^{k+m-2}+T & k,m \text{ are even} \\ mx^{k+m-2}+(k-1)x^{k+m-1}+x^{k-1}+T & k \text{ is odd}, m \text{ is even} \\ kx^{k+m-2}+(m-1)x^{k+m-1}+x^{m-1}+T & m \text{ is odd}, k \text{ is even} \\ (k+m-2)x^{k+m-1}+x^{m-1}+x^{k-1}+T & k,m \text{ are odd} \end{cases}.$$

This completes the proof. □

Finally, we compute the PI polynomial of the graphs with three strings. Using a similar argument as above, we have:

Theorem 2.3. The PI polynomial of G_i, $5 \leq i \leq 10$, are computed as follows:

$$PI(G_5,x) = tx^{k+m+n-1}+C(t+2,2)-t$$

$$PI(G_6,x) = \begin{cases} (m+k)x^{t-1}+nx^{t-2}+C(t,2) & n \text{ is even} \\ (m+k)x^{t-1}+(n-1)x^{t-1}+x^{n-1}+C(t,2) & n \text{ is odd} \end{cases},$$

$$PI(G_7,x) = PI(G_9,x) =$$

$$= \begin{cases} (n+m)x^{t-2}+s & n,m \text{ are even} \\ mx^{t-2}+(n-1)x^{t-1}+x^{n-1}+s & n \text{ is odd}, m \text{ is even} \\ nx^{t-2}+(m-1)x^{t-1}+x^{m-1}+s & m \text{ is odd}, n \text{ is even} \\ (m+n-2)x^{t-1}+x^{n-1}+x^{m-1}+s & n,m \text{ are odd} \end{cases}.$$

If k is even then:

$$PI(G_8,x) = \begin{cases} tx^{t-3}+w & n,m \text{ are even} \\ (m+k)x^{t-2}+nx^{t-1}+w & n \text{ is odd}, m \text{ is even} \\ (n+k)x^{t-2}+mx^{t-1}+w & m \text{ is odd}, n \text{ is even} \\ (m+n)x^{t-2}+kx^{t-1}+w & n,m \text{ are odd} \end{cases},$$

$$PI(G_{10},x) = \begin{cases} tx^{t-2}+w & n,m \text{ are even} \\ (m+k)x^{t-2}+(n-1)x^{t-1}+x^{n-1}+w & n \text{ is odd}, m \text{ is even} \\ (n+k)x^{t-2}+(m-1)x^{t-1}+x^{m-1}+w & m \text{ is odd}, n \text{ is even} \\ kx^{t-2}+(m+n-2)x^{t-1}+x^{n-1}+x^{m-1}+w & n,m \text{ are odd} \end{cases}.$$

If k is odd then:

$$PI(G_8,x) = \begin{cases} tx^{t-3}+w & n,m \text{ are odd} \\ (m+k)x^{t-2}+nx^{t-1}+w & m \text{ is odd}, n \text{ is even} \\ (n+k)x^{t-2}+mx^{t-1}+w & n \text{ is odd}, m \text{ is even} \\ (m+n)x^{t-2}+kx^{t-1}+w & n,m \text{ are even} \end{cases},$$

$$PI(G_{10},x) = \begin{cases} (m+n)x^{t-2}+(k-1)x^{t-1}+x^{k-1}+w & n,m \text{ are even} \\ mx^{t-2}+(n+k-2)x^{t-1}+x^{n-1}+x^{k-1}+w & n \text{ is odd}, m \text{ is even} \\ nx^{t-2}+(m+k-2)x^{t-1}+x^{m-1}+x^{k-1}w & m \text{ is odd}, n \text{ is even} \\ (t-3)x^{t-1}+x^{n-1}+x^{k-1}+x^{m-1}+w & n,m \text{ are odd} \end{cases}.$$

Where $t = k+m+n$, $s = kx^{t-1}+\frac{t(t-3)}{2}$ and $w = \frac{t^2-5t+2}{2}$.

3. Tables and Figures

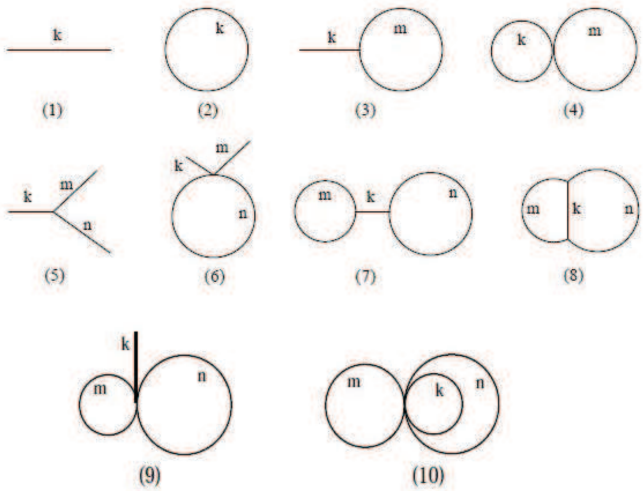

FIG. 3.1: Graphs from [4], including at most three strings

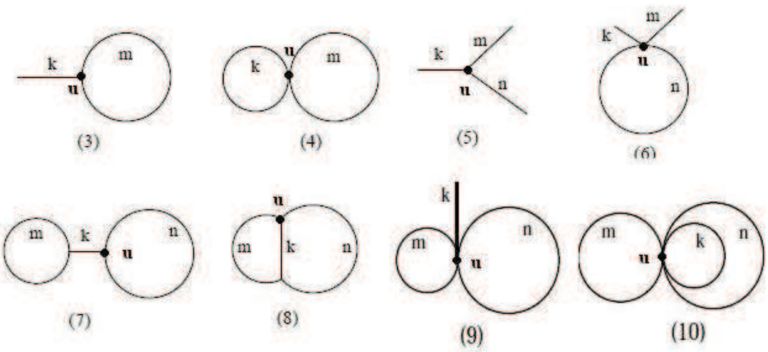

FIG. 3.2: Graphs G_i, $3 \leq i \leq 10$, with vertex u

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