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ON SZEGED POLYNOMIAL OF A GRAPH

A. R. ASHRAFI*, B. MANOOCHEHRIAN AND H. YOUSEFI-AZARI

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ABSTRACT. Suppose $e = uv$ is an edge connecting the vertices u and v of a graph G, $N_u(e|G)$ is the number of vertices of G lying closer to u and $N_v(e|G)$ is the number of vertices of G lying closer to v. Then the Szeged index of the graph G is defined as $Sz(G) = \sum_{e=uv\in E(G)} N_u(e|G)N_v(e|G)$.

In this paper, the notion of Szeged polynomial of a graph is introduced. We investigate some of the properties of this polynomial and compute it for some well-known graphs.

1. Introduction

Let G be a graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. As usual, the distance between the vertices u and v of G is denoted by $d(u, v)$ and it is defined as the number of edges in a minimal path connecting the vertices u and v. Throughout this article, we assume that G is connected.

A topological index is a numeric quantity from the structural graph of a molecule. Usage of topological indices in chemistry began in 1947 when chemist Harold Wiener developed the most widely known topological descriptor, the Wiener index, and used it to determine physical properties of types of alkanes known as paraffin [12]. Although the

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*Corresponding author

topological index, is easily calculable quantity, it does not uniquely correspond to the individual structure of a graph. It roughly represents the topological nature of the graph, i.e., branching and cyclization.

John Platt was the only person who immediately realized the importance of the Wiener's pioneering work and wrote papers analyzing and interpreting the physical meaning of the Wiener index.

We now describe some notations which will be kept throughout. A vertex weighted graph $G = (V, E, w)$ is a combinatorial object consisting of an arbitrary set $V = V(G)$ of vertices, a set $E = E(G)$ of unordered pairs $\{x, y\} = xy$ of distinct vertices of G called edges, and a weighting function w, where $w : V(G) \longrightarrow R$ assigns positive real numbers (weights) to vertices. The Cartesian product $G \times H$ of graphs G and H has the vertex set $V(G \times H) = V(G) \times V(H)$ and $(a, x)(b, y)$ is an edge of $G \times H$ if $a = b$ and $xy \in E(H)$, or $ab \in E(G)$ and $x = y$. If $G_1, G_2, \cdots, G_n$ are graphs then we denote $G_1 \times \cdots \times G_n$ by $\bigotimes_{i=1}^{n} G_i$.

Throughout this paper our notation is standard and taken mainly from [1, 2, 9, 10]. Let K_n, P_n, C_n, W_n denote the complete graph, path, cycle and wheel on n vertices, respectively. Also, Q_n is the cube of dimension n and $K_{m_1,\ldots,m_k}$ is a complete k-partite graph on parts of size $m_1, \ldots., m_k$. In the case of $r = 2$, we write $G = (V_1 + V_2, E)$ to denote a bipartite graph with parts V_1 and V_2.

2. **Definitions**

In this section, the notions of Szeged index, Szeged polynomial, and weighted hyper-Sz index are introduced. Szeged index is a mathematically elegant topological index defined by Ivan Gutman [4] at the Attila Jozsef University in Szeged, and so it was called the Szeged index, denoted by Sz. For more information about Szeged index we encourage the reader to consult [4, 7, 11] and references therein.

Definition 2.1. Suppose that $e = uv$ is an edge connecting the vertices u and v, $N_u(e|G)$ is the number of vertices of G lying closer to u and $N_v(e|G)$ is the number of vertices of G lying closer to v. Then *the Szeged index of the graph* G is defined as $Sz(G) = \sum_{e=uv \in E(G)} N_u(e|G) N_v(e|G)$.

In the previous definition, we notice that vertices equidistant from both ends of the edge $e = uv$ are not counted.

In 1988, Hosoya [5] introduced what he termed the Wiener polynomial of a graph as $H(G;x) = \sum_{k=1}^{l} d(G,k)x^k$, where $d(G,k)$ is the number of pairs of vertices in the graph G that are distance k apart, and l is the maximum value of k. In [8], Sagan et al., produced a treatment apparently independent of Hosoya's. Perhaps the most interesting property of $H(G,z)$ is that its first derivative, evaluated at x = 1, equals the Wiener index: $W(G) = H'(G,1)$.

In what follows, we continue the lines of [1, 2, 8, 12] to define the Szeged polynomial and weighted hyper-Sz index of a graph.

Definition 2.2. Let G be a connected graph, and let u, v be vertices of G and $e = uv$. Then *the Szeged polynomial of* G is defined as $\mathrm{Sz}(G;x) = \sum_{e=uv\in E(G)} x^{N_u(e|G)N_v(e|G)}$. If G is a vertex weighted graph then the Szeged polynomial of G is defined as follows

$$Sz_w(G,x) = \sum_{e=uv\in E(G)} w(u)w(v)x^{N_u(e|G)N_v(e|G)},$$

where $w(u)$ denotes the weight of vertex u.

Definition 2.3. Let G be a vertex weighted graph. Then *the weighted hyper-Sz index* G is defined as follows

$$Sz_w^{(2)}(G) = \sum_{e=uv\in E(G)} w(u)w(v)[N_u^2(e|G)N_v^2(e|G) + N_u(e|G)N_v(e|G)].$$

3. **Examples**

In this section we calculate the Szeged polynomial of some well-known graphs.

Example 3.1. Consider the complete graph K_n and the cycle graph C_n. Then $Sz(K_n,x) = \binom{n}{2}x$ and

$$Sz(C_n,x) = \begin{cases} nx^{n^2/4} & n \textit{ is even}, \\ nx^{(n-1)^2/4} & n \textit{ is odd}. \end{cases}$$

Example 3.2. In this example, the Szeged polynomial of the path P_n is computed. It is easy to see that $Sz(P_1.x) = 0$, $Sz(P_2,x) = x$ and

$Sz(P_3, x) = 2x^2$. If $n \geq 4$ then we have

$$\begin{aligned} Sz(P_n, x) &= x^{1\times n-1} + x^{2\times n-2} + \cdots + x^{n-1\times 1} \\ &= \begin{cases} 2x^{n-1} + 2x^{2(n-2)} + \cdots + x^{n/2\times n/2} & 2|n \\ 2x^{n-1} + 2x^{2(n-2)} + \cdots + 2x^{(n-1)/2\times(n+1)/2} & 2\not|n \end{cases}. \end{aligned}$$

Example 3.3. Suppose that W_n is the wheel graph with $n+1$ vertices. Then $Sz(W_n, x) = Sz(C_n, x) + nx^{1\times(n-3)}$ and by Example 3.1,

$$Sz(W_n, x) = \begin{cases} nx^{n-3} + nx^{n^2/4} & n \textit{ is even} \\ nx^{n-3} + nx^{(n-1)^2/4} & n \textit{ is odd.} \end{cases}$$

Example 3.4. Consider a complete r-partite graph $G = K_{n_1,n_2,\ldots,n_r}$ containing $v = |V(G)|$ vertices. By definition of this graph, Figure 1, $V = V(G)$ can be partitioned into subsets $V_1, V_2, ..., V_r$ of V such that for every i, $1 \leq i \leq r$, there is no edge between the vertices of V_i. In this graph we have $Sz(K_{n_1,n_2,\ldots,n_r}, x) = \sum_{1\leq i<j\leq r} n_i n_j x^{n_i n_j}$.

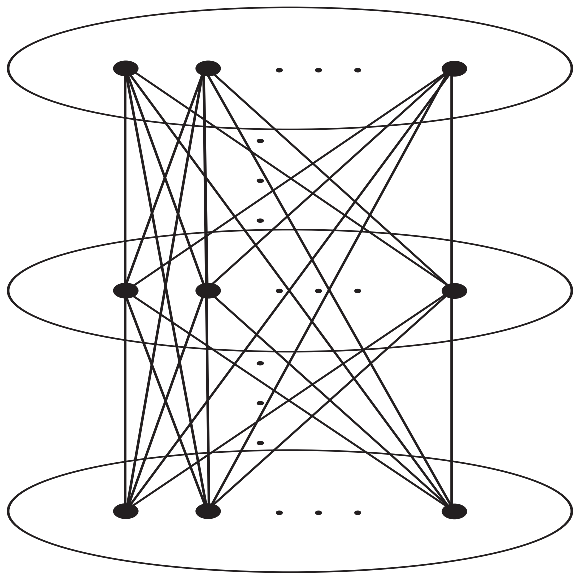

Figure 1. An r-partite graphs.

By the previous example, if G is a star with exactly $n+1$ vertices then $Sz(G, x) = nx^n$.

4. **Main results**

In this section, we prove Szeged polynomial of a graph has the same properties as Wiener polynomial of the graph under consideration. Also, some of the results of Sagan et al. are generalized to the case of Szeged polynomial of a graph, see [8] for details. We recall that a graph G is called bipartite if we can decompose the set of its vertices into two disjoint parts A and B such that no two vertices within the same set are adjacent. A bipartite graph is said to be balanced if $|A| = |B|$.

Lemma 4.1. *Let G be a connected graph with n vertices. Then we have*
(i) *$Sz(G,x)$ has the constant term 0 and $Sz(G;1) = |E(G)|$,*
(ii) *$Sz'(G;1) = Sz(G)$,*
(iii) *if T is a tree with edges e_1, ..., e_{n-1}, then $Sz(G;x) = \sum_{i=1}^{n-1} x^{n_i(n-n_i)}$, where n_i is the number of vertices of one component of $T - e_i$. Here $T - e_i$ is the subtree obtained from T by deleting the edge e_i. Moreover, the term with minimum degree of $Sz(T;x)$ is kx^{n-1}, in which k is the number of end vertices of T.*

Proof. The proof is straightforward and follows from the definition of Szeged polynomial. □

Corollary 4.2. *If $G = K_{n_1,n_2,\ldots,n_r}$ then*

$$Sz(K_{n_1,n_2,\ldots,n_r}) = \sum_{1\le i<j\le r} n_i^2 n_j^2.$$

Proof. The proof follows from Lemma 4.1 and Example 3.4. □

In what follows, we extend the main results of [1, 2, 13] to the Szeged polynomial of a weighted graph.

Theorem 4.3. $Sz_w^{(2)}(G) = 2Sz'_w(G,1) + Sz''_w(G,1)$.

Proof. By definition of Szeged polynomial, we have

$$\begin{aligned} Sz_w(G,x) &= \sum_{e=uv\in E(G)} w(u)w(v)x^{N_u(e|G)N_v(e|G)}, \\ xSz'_w(G,x) &= \sum_{e=uv\in E(G)} N_u(e|G)N_v(e|G)w(u)w(v)x^{N_u(e|G)N_v(e|G)} \\ & Sz'_w(G,x) + xSz''_w(G,x) \\ &= \sum_{e=uv\in E(G)} N_u(e|G)^2N_v(e|G)^2w(u)w(v)x^{N_u(e|G)N_v(e|G)-1}. \end{aligned}$$

Therefore, by definition of $Sz_w^{(2)}(G)$, one can see that

$$\begin{aligned} Sz_w^{(2)}(G) &= \sum_{e=uv\in E(G)} w(u)w(v)[N_u(e|G)^2N_v(e|G)^2 + N_u(e|G)N_v(e|G) \\ &= 2Sz'_w(G,1) + Sz''_w(G,1). \end{aligned}$$

This completes the proof. □

Suppose $G = (V_1 + V_2, E)$ denotes a bipartite graph whose partition has the parts V_1 and V_2. Then G is called balanced, if $|V_1| = |V_2|$. In what follows $d_G(x)$ denotes the degree of a vertex x in the graph G.

Theorem 4.4. *Let G be a graph with an even number of vertices. Then $\deg(Sz(G;x)) \leq 1/4|V(G)|^2$. Moreover, suppose $G = (V_1 + V_2, E)$ is bipartite. Then the upper bound is attained if and only if G is balanced and there exists an edge $e = xy$ of $E(G)$ such that $d_G(x) = |V_1|$ and $d_G(y) = |V_2|$.*

Proof. It is well-known fact then if $x+y$ is constant then the maximum value of xy is $[x^2/4]$, where [x] denotes the greatest integer $\leq x$. Since V(G) is even, $\deg(Sz(G;x)) \leq 1/4|V(G)|^2$. Suppose $G = (V_1 + V_2, E)$ is bipartite. If G is balanced and there exists an edge $e = uv$ such that $d_G(u) = |V_1|$ and $d_G(v) = |V_2|$ then $N_u(e|G)N_v(e|G) = |V_1||V_2|$ and by the first part of theorem $\deg(Sz(G;x)) = 1/4|V(G)|^2$. Conversely, we assume that $\deg(Sz(G;x)) = 1/4|V(G)|^2$. By the assumption, $|V| = |V_1|+|V_2|$ and $|V_1||V_2| = 1/4|V|^2$. So, $|V_1| = |V_2| = 1/2|V|$ and therefore G is balanced. On the other hand, since $\deg(Sz(G;x)) = 1/4|V(G)|^2$, there exists an edge $e = xy$ of $E(G)$ such that $d_G(x) = N_x(e|G) = |V_1|$ and $d_G(y) = N_y(e|G) = |V_2|$. □

Suppose that A and B are two disjoint n-cycles, and n is odd. Construct a graph G by connecting a vertex of A to a vertex of B. Then G is not bipartite, but $\deg(Sz(G;x)) = 1/4|V(G)|^2$.

Question. Suppose G is a graph with an even number of vertices and $\deg(Sz(G;x)) = 1/4|V(G)|^2$. What we can say about the structure of G?

Theorem 4.5. *Let G be a graph with an odd number of vertices. Then $\deg(Sz(G;x)) \leq 1/4(|V(G)|^2 - 1)$. Moreover, suppose that $G = (V_1 + V_2, E)$ is bipartite. Then the upper bound is attained if and only if $||V_1| - |V_2|| = 1$ and there exists an edge $e = xy$ of $E(G)$ such that $d_G(x) = |V_1|$ and $d_G(y) = |V_2|$.*

Proof. The proof is similar to Theorem 4.4. □

A similar argument shows that for an r-partite graph G, the upper bound is attained if and only if $r = 2$ and G satisfies the conditions of Theorem 4.4 or 4.5, when $|V|$ is even or odd. Trees and hexagonal systems are two of most important classes of bipartite graphs and Theorems 4.4 and 4.5 compute the degree of Szeged polynomial of such graphs.

In what follows we extend a result of Klavzar, Rajapakse and Gutman [7] to Szeged polynomial.

Theorem 4.6. *Let G and H be connected graphs. Then $Sz(G \times H, x) = |V(G)|Sz(H, x^{|V(G)|^2}) + |V(H)|Sz(G, x^{|V(H)|^2})$.*

Proof. Suppose that $P = G \times H$. There are only two types of edges in P corresponding to copies of G and of H, respectively. Let $(u, v) = ((a, x), (b, y))$ be an arbitrary edge of P. The Szeged polynomial of P can be written as follows:

$$\begin{aligned} Sz(P, x) &= \sum_{a \in V(G)} \sum_{xy \in E(H)} x^{N_u((a,x)(a,y)|P) N_v((a,x)(a,y)|P)} \\ &+ \sum_{x \in V(H)} \sum_{ab \in E(G)} x^{N_u((a,x)(b,x)|P) N_v((a,x)(b,x)|P)}. \end{aligned}$$

It is clear that $N_u((a, x)(a, y)|P) = |V(G)|N_x(xy|H)$ and $N_v((a, x)(a, y)|P) = |V(G)|N_y(xy|H)$. Analogous statements hold for the edge $(a, x)(b, x)$. Then

$$\begin{aligned} Sz(P,x) &= \sum_{a\in V(G)}\sum_{xy\in E(H)} x^{|V(G)|N_x(xy|H)|V(G)|N_y(xy|H)} \\ &+ \sum_{x\in V(H)}\sum_{ab\in E(G)} x^{|V(H)|N_a(ab|G)|V(H)|N_b(ab|G)} \\ &= |V(G)|\sum_{xy\in E(H)} (x^{|V(G)|^2})^{N_x(xy|H)N_y(xy|H)} \\ &+ |V(H)|\sum_{ab\in E(G)} (x^{|V(H)|^2})^{N_a(ab|G)N_b(ab|G)} \\ &= |V(G)|Sz(H,x^{|V(G)|^2}) + |V(H)|Sz(G,x^{|V(H)|^2}). \end{aligned}$$

This completes the proof. □

We conclude the paper by extending the previous theorem to product of n connected graphs.

Theorem 4.7. *Let $G_1, G_2, \cdots G_n$ be connected graphs. Then* $Sz(\otimes_{i=1}^n G_i, x) = \sum_{i=1}^n Sz(G_i, x^{\prod_{j=1,j\neq i}^n |V(G_j)|^2}) \prod_{j=1,j\neq i}^n |V(G_j)|$.

Proof. Since the product of connected graphs are connected [6], we can use induction. In Theorem 4.6, we proved the case of $n = 2$. Suppose that $G = \otimes_{i=1}^n G_1$, $H = \otimes_{i=1}^{n+1} G_i$ and the result is valid for G. Then we have

$$\begin{aligned} &Sz(H,x) = Sz(G\times G_{n+1},x) \\ &= |V(G)|Sz(G_{n+1},x^{|V(G)|^2}) + |V(G_{n+1})|Sz(G,x^{|V(G_{n+1})|^2}) \\ &= \prod_{i=1}^n |V(G_i)|Sz(G_{n+1},x^{\prod_{i=1}^n |V(G_i)|^2}) + |V(G_{n+1})|Sz(G,x^{|V(G_{n+1})|^2}) \\ &= \prod_{i=1}^n |V(G_i)|Sz(G_{n+1},x^{\prod_{i=1}^n |V(G_i)|^2}) \\ &+|V(G_{n+1})|\sum_{i=1}^n Sz(G_i,x^{\prod_{j=1,j\neq i}^n |V(G_j)|^2}) \prod_{j=1,j\neq i}^n |V(G_j)| \\ &= \sum_{i=1}^{n+1} Sz(G_i,x^{\prod_{j=1,j\neq i}^{n+1} |V(G_j)|^2}) \prod_{j=1,j\neq i}^{n+1} |V(G_j)|, \end{aligned}$$

as desired. □

Corollary 4.8. *If G is a connected graph then*

$$Sz(G^n, x) = \sum_{i=1}^{n} Sz(G, x^{|V(G)|^{2(n-1)}})|V(G)|^{n-1}.$$

Proof. The proof follows from Theorem 4.7. □

Suppose Q_n denotes an n-dimensional cube. Then we apply our previous corollary to compute the Szeged polynomial and then Szeged index of Q_n.

$$\begin{aligned} Sz(Q_n, x) &= Sz(K_2^n, x) = 2^{n-1}\sum_{i=1}^{n} Sz(K_2, x^{4^{n-1}}) \\ &= n2^{n-1}x^{4^{n-1}}. \end{aligned}$$

Thus, $Sz(Q_n) = Sz'(Q_n, 1) = n2^{3(n-1)}$.

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A. R. Ashrafi
Department of Mathematics
Faculty of Science
University of Kashan
Kashan 87317-51167, Iran
e-mail: ashrafi@kashanu.ac.ir

B. Manoochehrian
Academic Center for Education
Culture and Research
Tehran Branch
Tehran, Iran
e-mail: behzad@khayam.ut.ac.ir

H. Yousefi-Azari
School of Mathematics
Statistics and Computer Science
University of Tehran
Tehran, Iran
e-mail: hyousefi@ut.ac.ir