



Szeged index, edge Szeged index, and semi-star trees

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ABSTRACT

A semi-star tree is a star tree whose some edges may be replaced by paths of length more than one. In this paper we present some increasing and decreasing transformations for Szeged index of the semi-star trees. Then we introduce palm semi-star tree and uniform semi-star tree and show that they are extremal with respect to the Szeged index and edge Szeged index. In addition, we investigate the relation between the Szeged index and edge Szeged index for all trees.

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1. Introduction

In theoretical chemistry molecular structure descriptors – also called topological indices – are used to understand physico-chemical properties of chemical compounds. By now there exist a lot of different types of such indices which capture different aspects of the molecular graphs associated with the molecules considered.

A topological index of a graph G is a numerical invariant of G . The Wiener index is the first topological index defined by Wiener [15]. Mathematical properties and chemical applications of the Wiener index have been intensively studied in the past 30 years [1,2,6,4].

The Szeged index is another topological index introduced by Ivan Gutman [7]. In [12] the vertex PI index and Szeged index of bridge graphs have been determined [13]. In [11], the edge Szeged index of the Cartesian product of graphs has been computed. In [10] a matrix method to obtain exact formulae for computing the Szeged index of join and composition of graphs has been applied. In [2] an introduction to the theory of the Wiener index and a systematic survey of various Wiener-type topological indices and their interrelations have been provided. In [14] some extensions of the Szeged index, which account for fragments and their chemical nature as well as for their 3D geometry have been presented. For more information about the Szeged index and its mathematical properties one should refer the articles [3,5,9]. In this paper, we investigate the Szeged index and edge Szeged index on semi-star trees. The rest of this paper is organized as follows. After some preliminaries in Section 2, we present an increasing and a decreasing transformation in Section 3. In Section 4, we find the lower bound and the upper bound of the Szeged index and edge Szeged index of semi-star trees in SS_n^m . In addition, we characterize the semi-star trees in SS_n^m whose indices are equal to the mentioned bounds.

2. Preliminaries

In this section, we introduce some definitions and notations which we use throughout this paper. Let $G = (V(G), E(G))$ be a simple connected graph. Suppose that x and y are two vertices of G , by $d(x, y)$ we mean the number of edges of the

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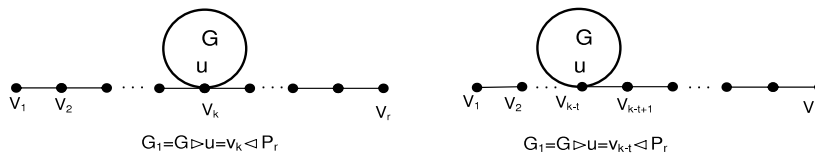


Fig. 1. Transformation.

shortest path connecting x and y . We call two vertices u and v to be neighbors if they are the endpoints of an edge e and we denote it by $e = uv$. The degree of vertex v is the number of its neighbor vertices. Suppose that $e = uv$ is an edge of G connecting the vertices u and v , the distance of e to a vertex $w \in V(G)$ is the minimum of the distances of its ends to w , that means $d(e, w) := \min\{d(w, u), d(w, v)\}$. Suppose that $W \subseteq V(G)$ by $d(e, W)$ we mean $\min\{d(e, w) : w \in W\}$. The number of vertices of G whose distance to the vertex u is smaller than the distance to the vertex v is denoted by $n_u(e)$. We also denote the number of edges of G whose distance to the vertex u is smaller than the distance to the vertex v by $m_u(e)$. In the other words, $n_u(e) := |\{x \in V(G) | d(x, u) < d(x, v)\}|$ and $m_u(e) := |\{f \in E(G) | d(f, u) < d(f, v)\}|$. The vertices and the edges of G with the same distance to u and v are not counted. The Szeged index of the graph G is defined as

$$Sz(G) = \sum_{e=uv \in E} n_u(e)n_v(e).$$

The edge Szeged index of the graph G is defined as

$$Sz_e(G) = \sum_{e=uv \in E} m_u(e)m_v(e).$$

A path in a graph is a sequence of distinct vertices $P : v_0 v_1 \dots v_k$ ($k \geq 1$), such that $v_i v_{i+1} \in E$ for each $i = 0, \dots, k - 1$. A leaf is a vertex of degree one.

A semi-star tree is a star tree whose some edges may be replaced by paths of length more than one. By SS_n^m we mean the set of semi-stars of order n with maximum degree m ($m \geq 3$). Obviously each tree T of SS_n^m has only one vertex of degree m . We call this vertex the center of T . If a path of a semi-star tree connects the center vertex to a leaf, we call it a pendant path. Let T be semi-star tree in SS_n^m . We call it a uniform semi-star tree if the length of its pendant paths are equal to $\lfloor \frac{n-1}{m} \rfloor$ or $\lceil \frac{n-1}{m} \rceil$. We denote it by $U_{n,m}$ and we call it a palm semi-star tree if it has a pendant path of length $n - m$. We denote it by $P_{n,m}$. Obviously $P_{n,m}$ has $m - 1$ pendant paths of length one.

In this paper, we investigate the Szeged index on semi-star trees. We shall present some increasing and decreasing transformations of Szeged index and edge Szeged index for semi-star trees. Then we shall find the upper bound and lower bound of Szeged index and edge Szeged index of semi-star trees in SS_n^m . Finally, we characterize the extremal semi-star trees in SS_n^m with respect to the Szeged index and edge Szeged index.

Let $G_1 = (V(G_1), E(G_1))$ and $G_2 = (V(G_2), E(G_2))$ be two graphs such that $V(G_1) \cap V(G_2) = \emptyset$. Suppose that $u \in V(G_1)$ and $v \in V(G_2)$. By $G_1 \triangleright u = v \triangleleft G_2$ we mean the obtained graph of identifying u and v . Suppose that v is a vertex of path $P : v_1 \dots v_r$. We define $d_l(v, P) := \min\{d(v, v_1), d(v, v_r)\}$ and call it the leaf distance of v with respect to P .

3. Transformations

In this section, we present a lemma that plays an important role in the main results of this paper. we may call this lemma as an increasing or a decreasing transformation, according to the leaf distance of the selected vertices of path for identifying.

Lemma 1. Let $G = (V, E)$ be a connected graph and $u \in V(G)$. Suppose that P_r be a non-trivial path graph, whose vertex set is disjoint from $V(G)$. Let v and w be two distinct vertices of P_r . If $d_l(v, P_r) < d_l(w, P_r)$ then $Sz(G \triangleright u = v \triangleleft P_r) > Sz(G \triangleright u = w \triangleleft P_r)$ (see Fig. 1).

Proof. Let us denote the difference between $d_l(v, P_r)$ and $d_l(w, P_r)$ by t . We assume without loss of generality that

$$d_l(v, P_r) = d(v, v_1) = k - t \tag{1}$$

and

$$d_l(w, P_r) = d(w, v_1) = k. \tag{2}$$

By the above assumptions, $v = v_{k-t}$ and $w = v_k$. Obviously,

$$\sum_{uv \in E(G)} n_u(e|G_1)n_v(e|G_1) = \sum_{uv \in E(G)} n_u(e|G_2)n_v(e|G_2),$$

we denote this value by x . Suppose that $|V(G - u)| = m$. Therefore,

$$\begin{aligned}
 Sz_v(G \triangleright u = w \triangleleft P_r) &= 1 \times (r + m - 1) + 2(r + m - 2) + \cdots + (k - t - 1)(r - k + t + m + 1) \\
 &\quad + (k - t)(r - k + t + m) + (k - t + 1)(r - k + m + t - 1) + \cdots \\
 &\quad + (k - 1)(r - k + m + 1) + (k + m)(r - k) + \cdots + (r - 1 + m) \times 1 + x. \\
 Sz_v(G \triangleright u = v \triangleleft P_r) &= 1 \times (r + m - 1) + 2(r + m - 2) + \cdots + (k - t - 1)(r - k + t + m + 1) \\
 &\quad + (k - t + m)(r - k + t) + (k - t + 1 + m)(r - k + t - 1) + \cdots \\
 &\quad + (k + m - 1)(r - k + 1) + (k + m)(r - k) + \cdots + (r - 1 + m) \times 1 + x. \\
 Sz_v(G \triangleright u = v \triangleleft P_r) - Sz_v(G \triangleright u = w \triangleleft P_r) &= (k - t + m)(r - k + t) + (k - t + m + 1)(r - k + t - 1) + \cdots + (k + m - 1)(r - k + 1) \\
 &\quad - [(k - t)(r - k + t + m) + (k - t + 1)(r - k + m + t - 1) + \cdots + (k - 1)(r - k + m + 1)] \\
 &= \sum_{i=0}^{t-1} (k - t + i + m)(r - k + t - i) - \sum_{i=0}^{t-1} (k - t + i)(r - k + t - i + m) \\
 &= \sum_{i=0}^{t-i} ((k - t + i + m)(r - k + t - i) - (k - t + i)(r - k + t - i + m)). \tag{3}
 \end{aligned}$$

By assumptions (1), (2), we have

$$r - k \geq k - 1. \tag{4}$$

Now if $0 \leq i \leq t - 1$ we conclude that:

$$\begin{aligned}
 r - k + t &\geq k - 1 + t \geq k + i \Rightarrow \\
 r - k + t - i &\geq k. \tag{5}
 \end{aligned}$$

According to the different values of i ($0 \leq i \leq t - 1$), we have at most four cases for the parentheses of Relation (3) which are listed below. For each case we test if it is valid.

Case 1 $k - t + m + i \leq r - k + t - i$ and $k - t + i \leq r - k + m + t - i$:

For the second inequality, if $k - t + i = r - k + m + t - i$ then $m \leq -m$, and this is a contradiction. Therefore the second inequality is always strict.

Case 2 $k - t + i + m \geq r - k + t - i$ and $k - t + i \leq r - k + t - i + m$:

The last inequality equivalent to $k - t + i - m \leq r - k + t - i$. Therefore, by this inequality and the first one we have

$$k - t + i - m \leq r - k + t - i \leq k - t + i + m.$$

Case 3 $k - t + i + m \geq r - k + t - i$ and $k - t + i \geq r - k + t - i + m$:

Therefore, in this case we have $r - k + t - i \leq k - t + i - m$. By this fact and Inequality (5), we conclude that $k \leq k - m - 1$. Since $m > 0$ this is a contradiction. That means this case never occur.

Case 4 $k - t + i + m \leq r - k + t - i$ and $k - t + i \geq r - k + t - i + m$:

Therefore, we have $k - t + i + m \leq r - k + t - i \leq k - t + i - m$, or $m \leq -m$. This case is also a contradiction. That means this case never occur too.

Note that, the product of two integer variables with given their sum increases if their difference decreases.

If we show that in the valid Cases 1 and 2 the value of the Summation (3) is greater than zero. To this end, we show that each term of summation is greater than zero. The proof is completed. It is sufficient to show that $(k - t + i + m)(r - k + t - i) > (k - t + i)(r - k + t - i + m)$ for each $i = 0, \dots, t - 1$.

On the other hand, the sum of two parentheses in the left side of this inequality is equal to the sum of two parentheses in the right side is equal to $r + m$. Therefore it is sufficient to show that the difference between two left side parentheses is smaller than difference between two right side parentheses. In the following, it is done for Cases 1 and 2, separately.

We now turn to *Case 1*:

$$(r - k + t - i) - (k - t + i + m) = r - 2k + 2t - 2i - m \tag{6}$$

$$(r - k + t - i + m) - (k - t + i) = r - 2k + 2t - 2i + m. \tag{7}$$

By the above argument, for completion the proof in this case, we only need to show that $r - 2k + 2t - 2i - m < r - 2k + 2t - 2i + m$, which is clear.

We now turn to *Case 2*:

$$(k - t + i + m) - (r - k + t - i) = m - (r - 2k + 2t - 2i) \tag{8}$$

$$(r - k + t - i + m) - (k - t + i) = m + (r - 2k + 2t - 2i). \tag{9}$$

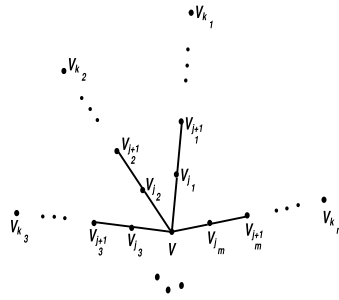


Fig. 2. A semi-star tree whose i th pendant path ($i = 1, \dots, m$) is a path of length $r_i = k_i - j_i + 1$. In $U_{n,m}$ the length of i th pendant path $r_i = \lfloor \frac{n-1}{m} \rfloor$ or $\lceil \frac{n-1}{m} \rceil$ for $i = 1, \dots, m$.

The proof is also completed in this case by showing that $m - (r + 2t - 2k - 2i) < m + (r + 2t - 2k - 2i)$. From (4) we have:

$$r - 2k \geq -1. \tag{10}$$

Since $0 \leq i \leq t - 1$ it follows that:

$$2t - 2i \geq 2. \tag{11}$$

From (10) and (11) we have $r - 2k + 2t - 2i \geq 1$. Therefore, $m - (r - 2k + 2t - 2i) < m + (r - 2k + 2t - 2i)$. That means $Sz(G \triangleright u = v \triangleleft P_r) > Sz(G \triangleright u = w \triangleleft P_r)$. \square

Corollary 1. Let $G = (V, E)$ be a connected graph and $u \in V(G)$. If $P_r : v_1, \dots, v_r$ is a path graph whose vertex set is disjoint from $V(G)$ then for each $k = 1, \dots, r$, $Sz(G \triangleright u = v \lceil \frac{r}{2} \rceil \triangleleft P_r) \leq Sz(G \triangleright u = v_k \triangleleft P_r)$.

4. Extremal semi-star trees and the bounds

In this section, we find the lower bound and the upper bound of the Szeged index and edge Szeged index of semi-star trees in SS_n^m . In addition, we characterize the semi-star trees in SS_n^m whose indices are equal to the mentioned bounds.

Szeged index

By the following lemma one can compute the Szeged index of a semi-star tree.

Lemma 2. If T is a semi-star in SS_n^m whose k th pendant path ($k = 1, \dots, m$) is a path of length r_k then

$$Sz(T) = \sum_{k=1}^m \sum_{i=1}^{r_k} i(n - i).$$

By the following theorem we characterize the semi-star tree in SS_n^m with the smallest Szeged index. We show that $U_{n,m}$ is the only smallest tree in SS_n^m with respect to the Szeged index (see Fig. 2).

Theorem 1. If T is a semi-star in SS_n^m then $Sz(T) \geq Sz(U_{n,m})$ with equality holding if and only if $T \cong U_{n,m}$.

Proof. For the sake of a contradiction we assume that $T \neq U_{n,m}$ is the smallest semi-star tree in SS_n^m with respect to the Szeged index whose center vertex is v .

It follows immediately that there exist two pendant paths $Q' : v = u_1 u_2 \dots u_r$ and $Q'' : v = w_1 w_2 \dots w_s$ in T , where $r - s > 1$. Let $P' = Q' - v, P'' = Q'' - v$ and let $G = T - \{u_2, u_3, \dots, u_r, w_2, w_3, \dots, w_s\}$.

We add a new vertex w ($w \notin V(T)$) and two new edges wu_2 and $w w_2$. In this case, $(P' \cup P'' + w) + \{wu_2, w w_2\}$ is the path $w_s w_{s-1} \dots w_2 w u_2 u_3 \dots u_r$ which we denote it by P . Obviously, $V(P) \cap V(G) = \emptyset$ and $T = G \triangleright v = w \triangleleft P$ and by Lemma 1, $Sz(T) > Sz(G \triangleright v = u_2 \triangleleft P)$. This is a contradiction. \square

Corollary 2. If T is a semi-star in SS_n^m then

$$Sz(T) \geq 2m/3 \left\lfloor \frac{n-1}{m} \right\rfloor^3 + 1/2(-nm + 3m - 2n + 2) \left\lfloor \frac{n-1}{m} \right\rfloor^2 + 1/6(6n^2 - 3mn + 5m - 18n + 12) \left\lfloor \frac{n-1}{m} \right\rfloor + (n-1)^2$$

with equality holding if and only if $T \cong U_{n,m}$.

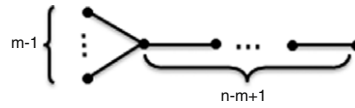


Fig. 3. The palm tree $P_{n,m}$.

Proof. By Lemma 2 one can show that

$$Sz(U_{n,m}) = 2m/3 \left\lfloor \frac{n-1}{m} \right\rfloor^3 + 1/2(-nm + 3m - 2n + 2) \left\lfloor \frac{n-1}{m} \right\rfloor^2 + 1/6(6n^2 - 3mn + 5m - 18n + 12) \left\lfloor \frac{n-1}{m} \right\rfloor + (n-1)^2$$

then according to Theorem 1 the claim follows. \square

By the following theorem we characterize the semi-star tree in SS_n^m with the largest Szeged index. We show that $P_{n,m}$ is the only largest tree in SS_n^m with respect to the Szeged index (see Fig. 3).

Theorem 2. If T is a semi-star in SS_n^m then $Sz(T) \leq Sz(P_{n,m})$ with equality holding if and only if $T \cong P_{n,m}$.

Proof. For the sake of a contradiction we assume that $T \neq P_{n,m}$ is the largest semi-star tree in SS_n^m with respect to the Szeged index whose center vertex is v .

It follows immediately that there exist two pendant paths $Q' : v = u_1u_2 \cdots u_r$ and $Q'' : v = w_1w_2 \cdots w_s$ in T , where $r, s \geq 2$. Let us assume without loss of generality that $r \leq s$. Let $P' = Q' - v$, $P'' = Q'' - v$ and let $G_1 = T - \{u_2, u_3, \dots, u_r, w_2, w_3, \dots, w_s\}$.

We add a new vertex $w (w \notin V(T))$ and two new edges wu_2 and ww_2 . In this case, $(P' \cup P'' + w) + \{wu_2, ww_2\}$ is the path $w_s w_{s-1} \cdots w_2 w u_2 u_3 \cdots u_r$ which we denote it by P . Obviously, $V(P) \cap V(G) = \emptyset$ and $T = G \triangleright v = w \triangleleft P$ and by Lemma 1, $Sz(T) < Sz(G \triangleright v = u_2 \triangleleft P)$. This is a contradiction. \square

Corollary 3. If T is a semi-star in SS_n^m then

$$Sz(T) \leq 1/6(2m^3 + n^3 - 3m^2n - 3m^2 + 9mn - 5m - 7n + 6)$$

with equality holding if and only if $T \cong P_{n,m}$.

Proof. By Lemma 2 one can show that

$$Sz(P_{n,m}) = 1/6(2m^3 + n^3 - 3m^2n - 3m^2 + 9mn - 5m - 7n + 6)$$

then according to Theorem 2 the claim follows. \square

Edge Szeged index

In the rest of this section we characterize the extremal semi-star trees with respect to the edge Szeged index. Moreover, we determine the lower bound and the upper bound of the edge Szeged index of semi-star trees.

Remark 1 ([8]). Assume that T is a tree, for any edge $e = (u, v)$ of $E(T)$, $m_u(e|T) = n_u(e|T) - 1$. Therefore

$$Sz_e(T) = \sum_{e=uv \in E(T)} [n_u(e|T) - 1][n_v(e|T) - 1].$$

In the following lemma, we show that the difference between $Sz(T)$ and $Sz_e(T)$ is fixed for every T in SS_n^m .

Lemma 3. If T is a tree, then $Sz(T) - Sz_e(T) = (n - 1)^2$.

Proof. There are $n - 1$ edges in $E(T)$. Therefore by Remark 1, we have

$$\begin{aligned} Sz(T) - Sz_e(T) &= \sum_{e=uv \in E(T)} n_u(e|T)n_v(e|T) - \sum_{e=uv \in E(T)} [n_u(e|T) - 1][n_v(e|T) - 1] \\ &= \sum_{e=uv \in E(T)} (n_u(e|T) + n_v(e|T) - 1) \\ &= \sum_{e \in E(T)} (n - 1) = (n - 1)(n - 1) = (n - 1)^2. \quad \square \end{aligned}$$

The extremal semi-star trees with respect to the edge Szeged index are characterized by the following theorems.

Theorem 3. *If T is a semi-star in SS_n^m then*

$$Sz_e(T) \geq 2m/3 \left\lfloor \frac{n-1}{m} \right\rfloor^3 + 1/2(-nm + 3m - 2n + 2) \left\lfloor \frac{n-1}{m} \right\rfloor^2 \\ + 1/6(6n^2 - 3mn + 5m - 18n + 12) \left\lfloor \frac{n-1}{m} \right\rfloor$$

with equality holding if and only if $T \cong U_{n,m}$.

Proof. By Theorem 1 and its corollary and Lemma 3 the assertion follows. \square

Theorem 4. *If T is a semi-star in SS_n^m then*

$$Sz_e(T) \leq 1/6(2m^3 + n^3 - 3m^2n - 3m^2 + 9mn - 5m - 7n + 6) - (n-1)^2$$

with equality holding if and only if $T \cong P_{n,m}$.

Proof. By Theorem 2 and its corollary and Lemma 3 the assertion follows. \square

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