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On Extremal Graphs of Weighted Szeged Index

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Abstract

An extension of the well-known Szeged index was introduced recently, named as *weighted Szeged index* ($wSz(G)$). This paper is devoted to characterizing the extremal trees and graphs of this new topological invariant. In particular, we proved that the star is a tree having the maximal $wSz(G)$. Finding a tree with the minimal $wSz(G)$ is not an easy task to be done. Here, we present the minimal trees up to 25 vertices obtained by computer and describe the regularities which retain in them. Our preliminary computer tests suggest that a tree with the minimal $wSz(G)$ is, at the same time, the connected graph of the given order that attains the minimal weighted Szeged index. Additionally, it is proven that among the bipartite connected graphs the complete balanced bipartite graph $K_{\lfloor n/2 \rfloor \lceil n/2 \rceil}$ attains the maximal $wSz(G)$. We believe that the $K_{\lfloor n/2 \rfloor \lceil n/2 \rceil}$ is a connected graph of given order that attains the maximum $wSz(G)$.

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1 Introduction

An idea that the structure of a molecule governs its physico–chemical properties is as old as modern chemistry. The problem of quantifying chemical structures was overcome by introducing the so-called molecular descriptors, which are the carriers of molecular structure information. These structural invariants are usually numbers or set of numbers. Nowadays, there are thousands of molecular descriptors that are commonly used in various disciplines of chemistry [1].

Topological indices are significant class among the molecular descriptors. The oldest and one of the most investigated topological indices is Wiener index, introduced in 1947 [2]. Although its definition is based on distances ($d(x,y)$) among pairs of vertices (x,y) in a graph G, in the seminal paper [2], Wiener used the following formula for its calculation:

$$W(T) = \sum_{e=\{uv\} \in E(T)} n_u(e) \cdot n_v(e) \tag{1}$$

where $n_u(e)$ is cardinality of the set $N_u(e = \{uv\}) = \{x \in V(G) : d(x,u) < d(x,v)\}$.

Formula (1) is valid only for acyclic molecules that are in chemical graph theory represented by trees. This fact triggered the introduction of a novel topological index, which definition coincides with Eq. (1), but its scope of usability is widen to all simple connected graphs. The name of this invariant is Szeged index, $Sz(G)$ [3] and it is defined as

$$Sz(G) = \sum_{e=\{uv\} \in E(G)} n_u(e) \cdot n_v(e) \tag{2}$$

Shortly after its introduction, Szeged index was attracted much attention in the mathematical chemistry community. Nowadays there is a vast literature presenting scientific researches deeply related to the Szeged index (e.g. for some recent results see [4–6] and references cited therein).

Inspired by an extension of the Wiener index, today known as degree distance [8, 9], Ilić and Milosavljević proposed a modification of the Szeged index [7] as a topological invariant that is worthy of investigations. This topological descriptor is named as *weighted Szeged index* and is defined as follows:

$$wSz(G) = \sum_{e=\{uv\} \in E(G)} [\deg(u) + \deg(v)] \cdot n_u(e) \cdot n_v(e) \tag{3}$$

where $\deg(u)$ is degree of the vertex u.

Half of decade has been passed since this invariant was introduced, but till today only some mediocre research activities involving $wSz(G)$ [10–12] were performed. Therefore, this paper contributes to the answering the elemental questions that are arising when someone works with a novel topological descriptor. In particular, the next section is reserved for the results and conjectures on graphs that are maximizing the $wSz(G)$, and the other one to the characterization of graphs that are minimizing it.

In the paper we will use the following definitions. By the *star graph* S_n we mean the complete bipartite graph $K_{1,n-1}$. We say that some vertex is an *internal leaf* of a graph G if this vertex becomes a leaf after removing all leaves of G. The subgraph of G induced by a set of vertices $B \subseteq V(G)$ is denoted by $G[B]$.

2 On graphs having maximum weighted Szeged index

The simplest connected graphs are trees and they are commonly used for the starting investigations of various properties and behaviors of novel topological descriptors. Thence, we are starting this section on graphs that are maximizing weighted Szeged index by characterizing a tree having maximum $wSz(G)$.

Theorem 1. *A tree with the maximum weighted Szeged index among n-vertex trees is the star graph S_n.*

Proof. Contrary to the statement in the Theorem 1, let us assume that there exists an extremal tree T with n vertices which is not a star. Since T is a non-star tree, there exists an edge uv of T such that u is an internal leaf and v is a non-leaf vertex of T. For the sake of simplicity, let us label $\deg(u)$ with a and $\deg(v)$ with b. Let $x_1, x_2, \ldots, x_{a-1}$ be the leaves attached at u. Also, let $y_1, y_2, \ldots, y_{b-1}$ be the neighbors of v distinct from u. We denote by Y_i the set of vertices of the $T - \{vy_i\}$ containing the vertex y_i. Without loss of generality, it is assumed that Y_1 is a biggest such set, i.e. $|Y_1| \geq |Y_i|$ for every $i > 1$.

Let us denote by A the set of vertices of the $T - v$ containing the vertex u and by $B = V(T) \setminus A$. Note that $|A| + |B| = n$, $|A| = a$, and $|A|, |B| \geq 2$.

It will be demonstrated that the transformation of a tree T into T', shown in Figure 1 (a contraction of the edge uv in the tree T into a leaf w in the tree T'), will always raise the $wSz(G)$, i.e. $\Delta := wSz(T') - wSz(T) > 0$.

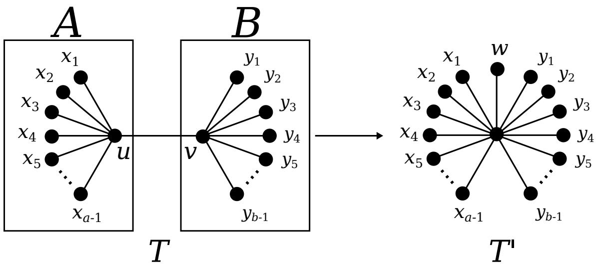


Figure 1

Note that the contribution of edges in $T[B - v]$ stays the same in $wSz(T')$ and $wSz(T)$. Thus, we can write

$$\Delta = \sum_{i=1}^{a-1}(b-1)n_{x_i}(x_iu)n_u(x_iu) + \sum_{i=1}^{b-1}(a-1)n_{y_i}(y_iv)n_v(y_iv) + (a+b)(n-1) - (a+b)|A||B| \ .$$

We know that $x_1, x_2, \ldots, x_{a-1}$ are leaves from which follows $n_{x_i}(x_iu) = 1$ for all i and $n_u(x_iu) = n - 1$. By a substitution we get

$$\Delta = (a-1)(b-1)(n-1) + (a-1)\sum_{i=1}^{b-1} n_{y_i}(y_iv)n_v(y_iv) + (a+b)(n-1) - a(a+b)(n-a) \ .$$

Now we want to argue that $\sum_{i=1}^{b-1} n_{y_i}(y_iv)n_v(y_iv)$ is minimal if $y_2, y_3, \ldots, y_{b-1}$ are leaves (the situation is depicted in Figure 2). Assume for contradiction that $|Y_i| > 1$ for some $i > 1$.

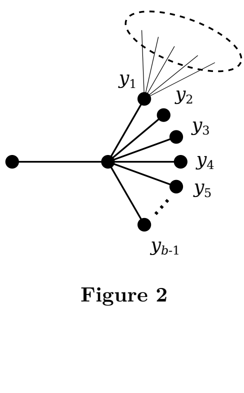


Figure 2

Observe that $\sum_{i=1}^{b-1}|Y_i| = n-a-1$. We know that

$$\sum_{i=1}^{b-1} n_{y_i}(y_i v) n_v(y_i v) = \sum_{i=1}^{b-1} |Y_i|(n-|Y_i|) = n\sum_{i=1}^{b-1}|Y_i| - \sum_{i=1}^{b-1}|Y_i|^2 .$$

Using a well known fact that $(x+1)^2+(y-1)^2 > x^2+y^2$ for $x>y$ and $x,y \in \mathbb{N}$, we conclude that $\sum_{i=1}^{b-1}|Y_i|^2$ attains the maximum value if $|Y_1| = n-a-b+1$ and $|Y_i| = 1$ for $1 < i \leq b-1$.

By using this fact we get that

$$\sum_{i=1}^{b-1} n_{y_i}(y_i v) n_v(y_i v) \geq (b-2)(n-1) + n(a+b-1) - (a+b-1)^2 ,$$

and thus

$$\Delta \geq (b-1)(a-1)(n-1) + (a-1)\left((b-2)(n-1) + n(a+b-1) - (a+b-1)^2\right)$$
$$+ (a+b)(n-1) - (a+b)a(n-a) \ .$$

It is enough to show that $\Delta' = 2bn - ab - b^2 + 3a + b - 4n + 2 > 0$, as $\Delta = (a-1)\Delta'$. For this, we distinguish three cases for the value of b. For $b=2$ and $b=3$ we obtain respectively

$$\Delta' = 4n - 2a - 4 + 3a + 2 - 4n + 2 = a$$

and

$$\Delta' = 6n - 3a - 9 + 3a + 3 - 4n + 2 = 2n - 4 \ .$$

Suppose now that $b \geq 4$. Together with an observation that $bn \geq b(a+b) = ab + b^2$ we obtain

$$\Delta' \geq bn - 4n + 3a + b + 2 > 0 \ .$$

This completes the proof. ■

Proposition 1. *Among all connected bipartite graphs the balanced complete bipartite graph $K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$ achieves the maximum weighted Szeged index.*

Proof. For an edge uv in a bipartite graph it holds that the $n_u + n_v = n$. Knowing this fact, it is obvious that

$$\max\,[n_u \cdot n_v] = \left\lfloor \frac{n^2}{4} \right\rfloor$$

Also it is well-known that the maximum number of edges in a bipartite graph is $\lfloor n^2/4 \rfloor$, and $\max\,[\deg(u)+\deg(v)] = n$. Then,

$$wSz(G) \leq n \cdot \left\lfloor \frac{n^2}{4} \right\rfloor^2 .$$

Equality holds if and only if $G \cong K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$. ■

Preliminary computer calculations indicate that the balanced complete bipartite graph has the maximal weighted Szeged index among all connected graphs. Taking into account this and the fact that the same graph is maximal for the ordinary Szeged index [13, 14], we believe that the following conjecture is true.

Conjecture 1. *For n-vertex graph the maximum weighted Szeged index is attained by the balanced complete bipartite graph* $K_{\lceil n/2 \rceil, \lfloor n/2 \rfloor}$.

After the submission of the paper to the journal, we were informed by Stijn Cambie that he managed to prove Conjecture 1.

3 On graphs having minimum weighted Szeged index

Problem of characterizing graphs with the minimal weighted Szeged index is more complex than with the graphs that maximizing it. Computer explorations of graphs having the minimal weighted Szeged index lead to the following conjecture:

Conjecture 2. *For n-vertex graphs the minimum weighted Szeged index is attained by a tree.*

Accepting the Conjecture 2 as true, we were pursuing for the minimal trees. The results of such computer search are presented in the Table 1.

Table 1. Trees from 7 to 25 vertices having minimum weighted Szeged index.

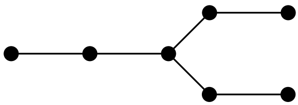
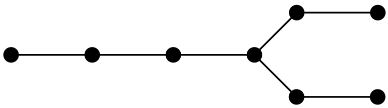
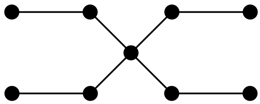
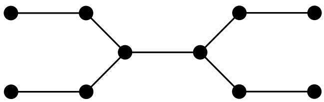
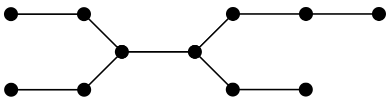
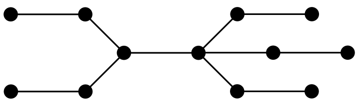
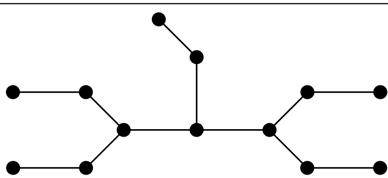
# vertices	Trees with minimal $wSz(G)$ index
7	
8	
9	
10	
11	
12	
13	

Table 1 continues on the next page

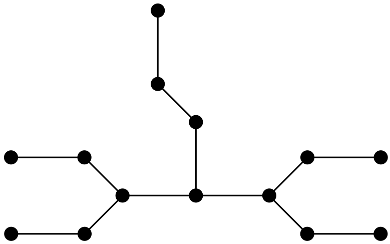
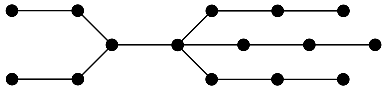
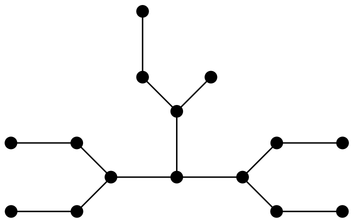
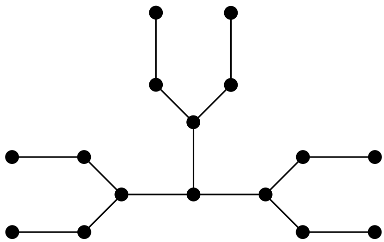
# vertices	Trees with minimal $wSz(G)$
14	
15	 
16	

Table 1 continues on the next page

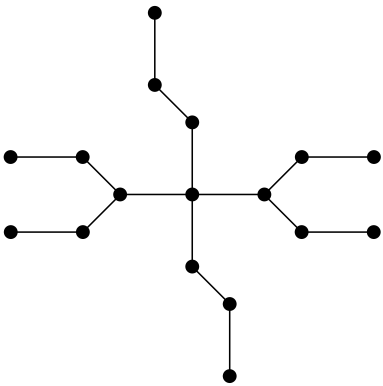
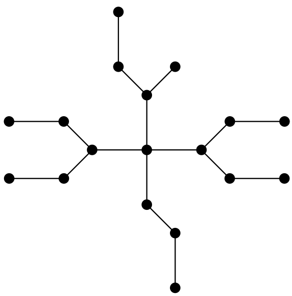
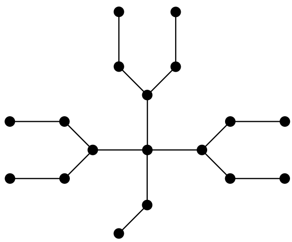
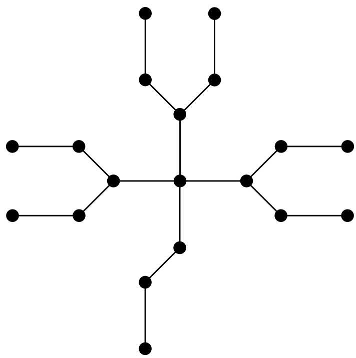
# vertices	Trees with minimal $wSz(G)$
17	
18	 
19	

Table 1 continues on the next page

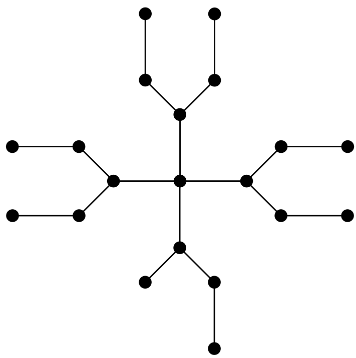
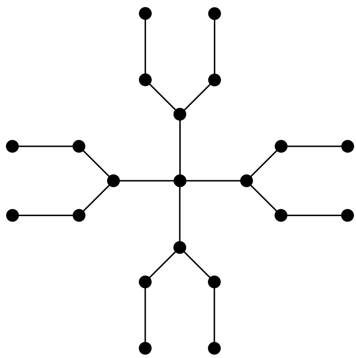
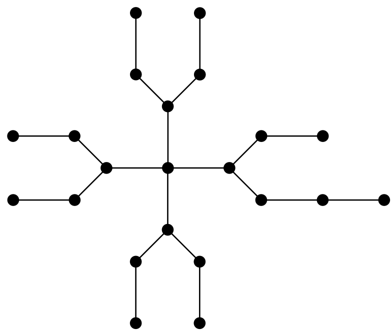
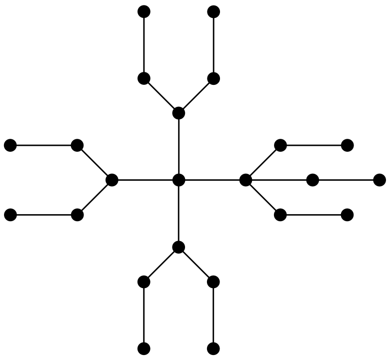
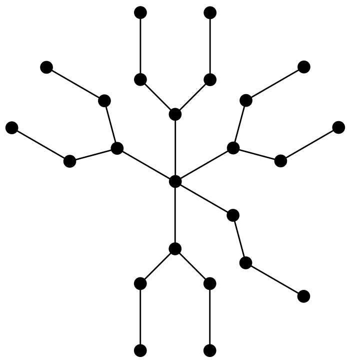
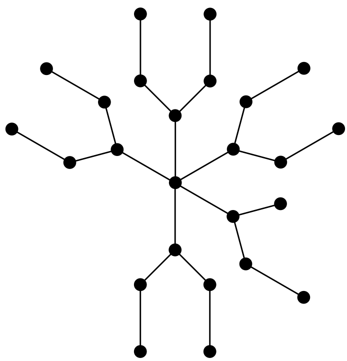
# vertices	Trees with minimal $wSz(G)$
20	
21	
22	

Table 1 continues on the next page

# vertices	Trees with minimal $wSz(G)$
23	
24	
25	

It is peculiar that some of the trees, shown in the Table 1, coincide with the minimal trees according to the well-know atom–bond connectivity index $ABC(T)$ [15]. In particular, minimal trees for the $wSz(T)$ and $ABC(T)$ for 7–13, 18, and 21 vertices are the same. It should be noted that apart from minimal trees shown here there may be other trees of the same order having either the minimal $ABC(T)$ or the minimal $wSz(T)$. Minimal trees, shown in the Table 1, mostly resemble to so-called Kragujevac trees introduced in [16].

The complete characterization of trees having minimal $wSz(T)$ is beyond our limits at the moment, but we noticed several regularities from figures in the Table 1 that will be outlined in the next subsection.

3.1 Some properties of trees having minimum weighted Szeged index

Here, we denote by $T_{\min}$ a tree with the minimum possible weighted Szeged index on n vertices, and study its properties. Notice that for some values of n, it may not be a uniquely defined tree.

Proposition 2. *For $n > 3$, no vertex of degree at least 6 in $T_{\min}$ is adjacent to two leaves.*

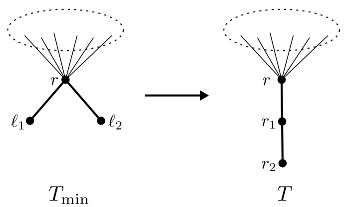


Figure 3. An illustration of construction in Proposition 2.

Proof. Suppose that a vertex r of $T_{\min}$ is a vertex of degree d adjacent to two leaves ℓ_1 and ℓ_2. Denote the vertices $N(v) \setminus \{\ell_1, \ell_2\}$ as $x_1, x_2, \ldots, x_{d-2}$ and the set of vertices of the components of $T_{\min} - vx_i$ containing x_i as X_i for all $i \in \{1, 2, \ldots, d-2\}$.

Define a new graph T as

$$V(T) = V(T_{\min}) - \ell_1 - \ell_2 + r_1 + r_2,$$

$$E(T) = E(T_{\min}) - r\ell_1 - r\ell_2 + rr_1 + r_1r_2.$$

It is easy to see that $\deg_{T_{\min}}(r) = \deg_T(r) + 1$ and $\sum_{i=1}^{d-2} |X_i| = n - 3$. Also, as in the proof of Theorem 1, the maximum possible value of $\sum_{i=1}^{d-2} |X_i|^2$ is $(d-3) + (n-d)^2$.

The difference $\Delta = wSz(T_{\min}) - wSz(T)$ can then be written as

$$\begin{aligned}\Delta &= \left(\sum_{i=1}^{d-2} |X_i| \cdot (n - |X_i|)\right) + 2(d+1)(n-1) - (d+1) \cdot 2 \cdot (n-2) - 3(n-1) \\ &\geq \left(\sum_{i=1}^{d-2} |X_i| \cdot (n - |X_i|)\right) + 2d - 3n + 5 = n \cdot (n-3) - \sum_{i=1}^{d-2} |X_i|^2 + 2d - 3n + 5 \\ &\geq n \cdot (n-3) - (n-d)^2 - (d-3) + 2d - 3n + 5 = 2dn - 6n - d^2 + d + 8\,.\end{aligned}$$

Since $d \geq 6$, it holds $dn \geq 6n$. Also, $dn \geq d^2$ and thus we conclude that $\Delta > 0$. This implies that T has smaller weighted Szeged index than $T_{\min}$, which is a contradiction.
■

Proposition 3. *No vertex of degree at least 10 in $T_{\min}$ is simultaneously incident with two 2-rays and a leaf.*

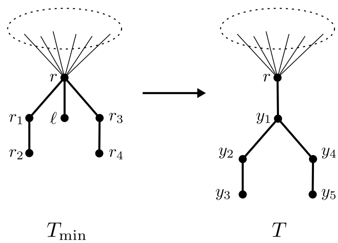


Figure 4. An illustration of construction in Proposition 3.

Proof. Suppose contradictory that $T_{\min}$ has a vertex r of degree d incident with two 2-rays and a leaf. Denote the vertices $N(r) \setminus \{r_1, r_3, \ell\}$ as $x_1, x_2, \ldots, x_{d-3}$ and the set of vertices of the components of $T_{\min} - rx_i$ containing x_i as X_i for all $i \in \{1, 2, \ldots, d-3\}$.

Define a new graph T as

$$V(T) = V(T_{\min}) - \{r_1, r_2, r_3, r_4, \ell\} \cup \{y_1, y_2, \ldots, y_5\},$$

$$E(T) = \big(E(T_{\min}) \cap E[V(T)]\big) \cup \{ry_1, y_1y_2, y_2y_3, y_1y_4, y_4y_5\}.$$

Observe that the contribution of the edges r_1r_2 and r_3r_4 to $wSz(T)$ is the same as the contribution of the edges y_2y_3 and y_4y_5 to $wSz(T_{\min})$. Also, the role of rr_1 and rr_3 is symmetric and the same holds for y_1y_2 and y_1y_4.

We now make a few observations, similar to those in Proposition 2. We see that $\deg_{T_{\min}}(r) = \deg_T(r) + 2$. Furthermore $\sum_{i=1}^{d-3} |X_i| = n - 6$. Also, by the same argument as in the proof of Theorem 1, the maximum value of $\sum_{i=1}^{d-3} |X_i|^2$ is $(n-d-2)^2 + d - 4$.

We claim that $\Delta = wSz(T_{\min}) - wSz(T) > 0$. We can write

$$\Delta = 2\left(\sum_{i=1}^{d-3} |X_i| \cdot (n - |X_i|)\right) + 2(2+d)(n-2)2 + (d+1)(n-1) - (d+1)(n-5)5$$
$$- 20(n-2) = 2\sum_{i=1}^{d-3} |X_i| - 2\sum_{i=1}^{d-3} |X_i|^2 + 2(2+d)(n-2)2 + (d+1)(n-1)$$
$$- (d+1)(n-5)5 - 20(n-2) \geq -2d^2 + 4dn + 6d - 20n + 48 \ .$$

Since $d \geq 10$ by our assumption, it holds that $2dn \geq 20n$ and also $2dn \geq 2d^2$. Thus, $\Delta > 0$ and we conclude that T has smaller weighted Szeged index than $T_{\min}$, which is a contradiction. ■

Proposition 4. *No vertex in $T_{\min}$ is incident to a 4-ray.*

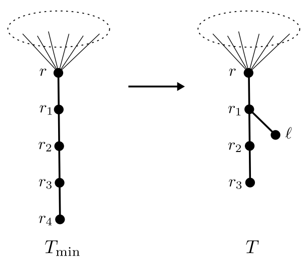


Figure 5. An illustration of construction in Proposition 4.

Proof. For $n \leq 6$, our computer search verified the claim. So assume that $n \geq 7$. Suppose that we have a vertex r of degree d in $T_{\min}$ incident to a 4-ray vertices $rr_1r_2r_3r_4$, as is shown in Figure 5. We define a new tree T in the following way.

$$V(T) = V(T_{\min}) - r_4 + \ell,$$
$$E(T) = E(T_{\min}) - r_3r_4 + r_1\ell \ .$$

We define $\Delta = wSz(T_{\min}) - wSz(T)$ and our aim is to show that $\Delta > 0$. By the definition of weighted Szeged index it suffices to calculate differences on the edges $\{r_1, r_2, r_3, r_4, r, \ell\}$. Also, the summand for the edge r_3r_4 in $wSz(T_{\min})$ is equal to the summand of the edge r_2r_3 in $wSz(T)$. Thus,

$$\Delta = ((d+2) \cdot 4 \cdot (n-4) + 4 \cdot 3 \cdot (n-3) + 4 \cdot 2 \cdot (n-2))$$
$$+ (-(d+3) \cdot 4 \cdot (n-4) - 4 \cdot (n-1) - 5 \cdot 2 \cdot (n-2))$$
$$= (4dn - 16d + 28n - 84) + (-4dn + 16d + 26n + 72) = 2n - 12.$$

Thus, $\Delta > 0$ for all $n \geq 7$. Therefore, $T_{\min}$ is not a tree with the minimum weighted Szeged index among n-vertex trees, a contradiction. ■

Proposition 5. *No vertex of degree 3 in* $T_{\min}$ *is adjacent to two 3-rays.*

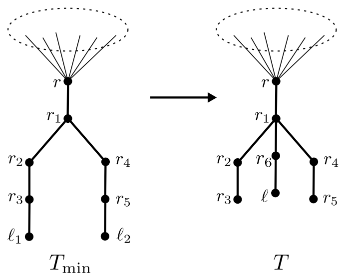


Figure 6. An illustration of construction in Proposition 5.

Proof. Suppose that the tree $T_{\min}$, shown in Figure 6, is a tree with minimal $wSz(T)$. Let us transform $T_{\min}$ to T in a way as it is illustrated in the Figure 6. In particular,

$$V(T) = V(T_{\min}) - \ell_1 - \ell_2 + r_6 + \ell$$
$$E(T) = E(T_{\min}) - r_3\ell_1 - r_5\ell_2 + r_1r_6 + r_6\ell\ .$$

We define $\Delta = wSz(T_{\min}) - wSz(T)$. By showing that $\Delta > 0$ proves that transformation, depicted in Figure 6, minimizes the $wSz(T)$. It is obvious that Δ depends only on edges that are existing among vertices $\{r, r_1, r_2, r_3, r_4, r_5, r_6, \ell, \ell_1, \ell_2\}$. Also, contributions of edges $r_3\ell_1$ and $r_5\ell_2$ in the $T_{\min}$ is equal to the contributions of edges r_2r_3 and r_4r_5 in the

T. We label the degree of the vertex r in $T_{\min}$ by d like in previous propositions. Thus,

$$\Delta = 2 \cdot [(2+2)\cdot 2 \cdot (n-2) + (2+3)\cdot 3 \cdot (n-3)] + (d+3)\cdot 7 \cdot (n-7)$$

$$- 3 \cdot [(2+4)\cdot 2 \cdot (n-2)] - (1+2)\cdot (n-1) - (d+4)\cdot 7 \cdot (n-7)$$

$$= 30(n-3) - 20(n-2) - 3(n-1) - 7(n-7) = 2 > 0 \ .$$

We obtained that for all $n > 7$ the $\Delta > 0$. This indicates that our assumption that $T_{\min}$ is a tree with minimum $wSz(T)$ is false, i.e. the transformation given in Figure 6 is minimizing the weighted Szeged index. ■

4 Conclusion

We have been examining the extremal graphs with respect to weighted Szeged index. It has been proven that the star graph has the maximum value of the $wSz(T)$ among all trees. In addition, among all bipartite graphs, the balanced complete bipartite graph achieves the maximum value of the weighted Szeged index. We failed to characterize graph (or graphs) that has the maximum $wSz(G)$ among all connected graphs. Based on a computer investigation, it is believed that it would be the balanced complete bipartite graph (see Conjecture 1).

Characterizing a graph (or graphs) that is (are) minimizing weighted Szeged index is more complex than finding those with maximum value. We are convinced that among all connected graphs it must be a tree (see Conjecture 2). Then, the minimal trees with respect to $wSz(T)$ obtained by computer and some of their properties are presented.

Proving Conjectures 1 and 2 and characterizing corresponding graphs remains a task for future research endeavors.

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