# On the difference between the revised Szeged index and the Wiener index

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#### Abstract

Let  $Sz^{\star}(G)$  and W(G) be the revised Szeged index and the Wiener index of a graph G. Chen, Li, and Liu [European J. Combin. 36 (2014) 237–246] proved that if G is a non-bipartite connected graph of order  $n \geq 4$ , then  $Sz^{\star}(G) - W(G) \geq (n^2 + 4n - 6)/4$ . Using a matrix method we prove that if G is a non-bipartite graph of order n, size m, and girth g, then  $Sz^{\star}(G) - W(G) \geq n \left(m - \frac{3n}{4}\right) + P(g)$ , where P is a fixed cubic polynomial. Graphs that attain the equality are also described. If in addition  $g \geq 5$ , then  $Sz^{\star}(G) - W(G) \geq n \left(m - \frac{3n}{4}\right) + (n - g)(g - 3) + P(g)$ . These results extend the bound of Chen, Li, and Liu as soon as  $m \geq n+1$  or  $g \geq 5$ . The remaining cases are treated separately.

Key words: Wiener index; Szeged index; revised Szeged index; isometric cycle

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### 1 Introduction

The Wiener index W(G) of a graph G forms a landmark in mathematical chemistry for the extensive investigation in the last decades of the so-called topological indices. The developed theory offers numerous useful tools to chemists and is also of independent interest in discrete mathematics and wider. Being equivalent to the average distance of a graph, the Wiener index is actually one of the most natural concepts in metric graph theory, in particular it is an important measure for (large) networks. Despite the long history of investigations, the Wiener index is still a hot research topics, cf. [4, 6, 14, 15].

Numerous variations and extensions of the Wiener index have been proposed by now, cf. [24]. One of the most prolific variants is the Szeged index Sz(G) of G, see the survey [7], the recent paper [11], and references therein. The Szeged index sums contributions of all the edges of a given graph, where for a fixed edge e = uv, vertices closer to u and vertices closer to v are treated. If G is bipartite, then all of its vertices are involved in the definition of Sz(G), but as soon G contains odd cycles, some vertices do not contribute (to a given edge).

In order that (for a given edge) all vertices would contribute to an invariant, the revised Szeged index  $Sz^*$  was proposed in [23]; it was named there the revised Wiener index. As expected,  $Sz^*(G) = Sz(G)$  holds for any bipartite graph G. The present name for  $Sz^*$  was coined in [21], where it was used to measure network bipartivity. At about the same time, relationships between the Wiener index, the Szeged index and the revised Szeged index were studied on tree-like graphs in [22]. Extremal graphs with respect to the revised Szeged index in unicyclic graphs and in bicyclic graphs were studied in [26] and [17], respectively. The revised Szeged index of hierarchical product of graphs was investigated in [25], while in [5] a new formula for computing this invariant is presented. For a normalized version of the revised Szeged index see [1].

Since  $Sz(G) \ge W(G)$  holds for any connected graph [13],  $Sz^*(G) \ge W(G)$  holds as well. But how large the difference  $Sz^*(G) - W(G)$  can be? Chen, Li, and Liu proved the following result which confirms a conjecture that was presented at the talk [9] and is due to the computer program AutoGraphiX.

**Theorem 1.1** [2, Theorem 4.3] If G is a non-bipartite, connected graph with  $n \ge 4$  vertices, then

$$Sz^{\star}(G) - W(G) \ge \frac{n^2 + 4n - 6}{4}$$
.

Moreover, the bound is best possible when the graph is composed of a cycle  $C_3$  and a tree T on n-2 vertices sharing a single vertex.

The bound of theorem depends only on the order of a given graph. On the other

hand, the Wiener index and the revised Szeged index of a graph are functions of its metric structure. This motivated us to search for an alternative lower bound that would involve also the size of a graph. Since for bipartite graphs G,  $Sz(G) = Sz^*(G)$ , and the difference between the Szeged index and the Wiener index was studied in[12, 19, 20], we focus in this paper on non-bipartite graphs. Our main results are presented in Theorems 2.3 (for general non-bipartite graphs) and 3.5 (for non-bipartite graphs of girth at least 5). A consequence of the first main result is that if G is a non-bipartite graph of order n, size m, and girth g, then

$$Sz^{\star}(G) - W(G) \ge n\left(m - \frac{3n}{4}\right) + P(g),$$

where for an integer t,

$$P(t) = \begin{cases} \frac{t}{2} \left( (t/2)^2 - 2 \right); & t \text{ even }, \\ \frac{t}{2} \left( \frac{t-1}{2} \right) \left( \frac{t-3}{2} \right); & t \text{ odd }. \end{cases}$$

A similar but stronger result holds when the girth of G is at least 5. In the concluding section we observe that our results extend the bound of Theorem 1.1 as soon as one of the conditions  $m \ge n + 1$  and  $g \ge 5$  holds and treat the remaining cases when m = n and g = 3, 4.

### 2 Preliminaries

In this section we recall definitions, concepts, and results needed in this paper.

The Wiener index of a (connected) graph G is  $W(G) = \sum_{\{u,v\}\subseteq V(G)} d(u,v)$ , where d(u,v) is the usual shortest-path distance between u and v. If G is a connected graph and  $e = uv \in E(G)$ , then set

$$N_u(e) = \{x \in V(G) : d(x, u) < d(x, v)\},\$$
  

$$N_v(e) = \{x \in V(G) : d(x, u) > d(x, v)\},\$$
  

$$N_0(e) = \{x \in V(G) : d(x, u) = d(x, v)\}.\$$

Clearly, these three sets form a partition of V(G). Note also that  $N_0(e) = \emptyset$  holds for any edge e of a bipartite graph G. Set in addition  $n_u(e) = |N_u(e)|$ ,  $n_v(e) = |N_v(e)|$ , and  $n_0(e) = |N_0(e)|$ . Then the revised Szeged index of G is:

$$Sz^{\star}(G) = \sum_{e=uv \in E(G)} \left( n_u(e) + \frac{n_0(e)}{2} \right) \left( n_v(e) + \frac{n_0(e)}{2} \right)$$

We will also use the *vertex PI index* of G, an invariant introduced in [10] (see also [16] and references therein) as follows:

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

If x is a vertex of a (connected) graph G, then let

$$m_x = |\{e = uv \in E(G) : d(x, u) \neq d(x, v)\}|.$$

The following result follows by a double counting of the ordered pairs  $(x, e), x \in V(G)$ ,  $e = uv \in E(G)$ , for which  $d(x, u) \neq d(x, v)$ .

**Lemma 2.1** [18, Lemma 2] If G be a connected graph, then  $PI_v(G) = \sum_{x \in V(G)} m_x$ .

Lemma 2.1 in particular implies (for each vertex x consider a BFS-free rooted in x) that  $PI_v(G) \ge n(n-1)$ . For the class of graphs  $X_n$  that attain this bound see [18, Theorem 2]. The following lemma also easily follows by considering a BFS-tree rooted at u.

**Lemma 2.2** [2, Lemma 4.2] Let G be a non-bipartite, connected graph of order  $n \ge 4$ and size  $m \ge n$ . Then for every vertex  $u \in V(G)$ , there exists an edge  $e \in E(G)$  such that  $u \in N_0(e)$ .

To conclude these preliminaries we recall the main result of [12].

**Theorem 2.3** [12, Theorem 3.2] If G is a connected graph of order  $n \ge 5$  and girth  $g \ge 5$ , then

$$Sz(G) - W(G) \ge PI_v(G) - n(n-1) + (n-g)(g-3) + P(g),$$

where

$$P(g) = \begin{cases} \frac{g}{2} \left( (g/2)^2 - 2 \right); & g \text{ even}; \\ \frac{g}{2} \left( \frac{g-1}{2} \right) \left( \frac{g-3}{2} \right); & g \text{ odd}. \end{cases}$$

### 3 New estimates

We now extend Theorem 1.1 as follows. Here P is the cubic polynomial as introduced in Section 1, see also Theorem 2.3.

**Theorem 3.1** If G is a non-bipartite graph of order n, size m, and girth g, then

$$Sz^{\star}(G) - W(G) \geq nm - n(n-1) + P(g) + \frac{2n-5}{4} \sum_{e \in E(G)} n_0(e) - \frac{1}{2} \sum_{e \in E(G)} {\binom{n_0(e)}{2}}.$$

**Proof.** Let  $V(G) = \{x_1, \ldots, x_n\}$ ,  $E(G) = \{e_1, \ldots, e_m\}$ , and let Y be an ordered list of all  $\binom{n}{2}$  unordered pairs of vertices of G. Define the matrix  $B = [b_{ij}]$  of dimension  $\binom{n}{2} \times m$  as follows. Its rows correspond to the elements of Y, its columns to the elements of E(G). If the row *i* corresponds to the pair  $\{x, y\}$  and the column *j* to the edge  $e_j = uv$ , then set

$$b_{ij} = \begin{cases} 1; & \{x, y\} \cap \{u, v\} = \emptyset \text{ and} \\ & (x \in N_u(e_j) \text{ and } y \in N_v(e_j)) \text{ or } (x \in N_v(e_j) \text{ and } y \in N_u(e_j)), \\ \frac{1}{2}; & (x \in N_u(e_j) \text{ and } y \in N_0(e_j)) \text{ or} \\ & (x \in N_0(e_j) \text{ and } y \in N_v(e_j)) \text{ or} \\ & (x, y \in N_0(e_j)), \\ 0; & \text{otherwise}. \end{cases}$$

Note that the sum of the entries of the  $j^{th}$  column is equal to

$$(n_u(e_j) - 1)(n_v(e_j) - 1) + \frac{1}{2}n_0(e_j)(n_u(e_j) + n_v(e_j)) + \frac{1}{2}\binom{n_0(e_j)}{2}$$

Setting

$$\beta = \sum_{i=1}^{\binom{n}{2}} \sum_{j=1}^{m} b_{ij}$$

we thus obtain:

$$\beta = \sum_{j=1}^{m} \left[ (n_u(e_j) - 1)(n_v(e_j) - 1) + \frac{1}{2}n_0(e_j)(n_u(e_j) + n_v(e_j)) + \frac{1}{2}\binom{n_0(e_j)}{2} \right]$$

$$= \sum_{j=1}^{m} \left[ n_u(e_j)n_v(e_j) + \frac{1}{2}n_u(e_j)n_0(e_j) + \frac{1}{2}n_v(e_j)n_0(e_j) + \frac{1}{4}n_0(e_j)^2 \right]$$

$$- \sum_{j=1}^{m} \left[ n_u(e_j) + n_v(e_j) \right] - \frac{1}{4}\sum_{j=1}^{m} n_0(e_j) + m$$

$$= Sz^*(G) - PI_v(G) - \frac{1}{4}\sum_{j=1}^{m} n_0(e_j) + m.$$
(1)

Let  $\mu_{x,y}$  and  $\lambda_{x,y}$  be the number of entries of the row of *B* corresponding to the pair  $\{x, y\}$  containing 1 and 1/2, respectively. Then

$$\beta = \sum_{\{x,y\}} \mu_{x,y} + \frac{1}{2} \sum_{\{x,y\}} \lambda_{x,y} \,. \tag{2}$$

If we set

$$\mu'_{x,y} = \begin{cases} \mu_{x,y} - d(x,y) + 2; & d(x,y) \ge 2, \\ \mu_{x,y}; & \text{otherwise}, \end{cases}$$

then we have

$$\sum_{\{x,y\}\in\binom{V(G)}{2}}\mu_{x,y} = \sum_{\substack{\{x,y\}\\xy\notin E(G)}}\mu_{x,y} + \sum_{\substack{\{x,y\}\\xy\notin E(G)}}\mu_{x,y} \\ = \sum_{\substack{\{x,y\}\\xy\notin E(G)}}(\mu'_{x,y} + d(x,y) - 2) + \sum_{\substack{\{x,y\}\\xy\in E(G)}}\mu'_{x,y} \\ = \sum_{\substack{\{x,y\}\\xy\in E(G)}}\mu'_{x,y} + (W(G) - m) - 2\left(\binom{n}{2} - m\right) \\ = \sum_{\substack{\{x,y\}}}\mu'_{x,y} + W(G) + m - n(n-1).$$
(3)

On the other hand, for a vertex x of G set

$$m'_x = |\{e \in E(G) : x \in N_0(e)\}|,$$

and for a pair of vertices  $\{x,y\}$  let

$$m'_{x,y} = |\{e \in E(G) : x, y \in N_0(e)\}|.$$

Then it follows by the inclusion-exclusion principle that for a pair of vertices x and y we have  $\lambda_{x,y} = m'_x + m'_y - m'_{x,y}$ . Therefore,

$$\sum_{\{x,y\}\in \binom{V(G)}{2}} \lambda_{x,y} = \sum_{\{x,y\}\in \binom{V(G)}{2}} \left[ m'_x + m'_y - m'_{x,y} \right] \\ = (n-1) \sum_{x\in V(G)} m'_x - \sum_{\{x,y\}\in \binom{V(G)}{2}} m'_{x,y}.$$
(4)

Combining (3) and (4) with (2) we obtain

$$\beta = \sum_{\{x,y\}} \mu'_{x,y} + W(G) + m - n(n-1) + \frac{n-1}{2} \sum_{x \in V(G)} m'_x - \frac{1}{2} \sum_{\{x,y\} \in \binom{V(G)}{2}} m'_{x,y},$$
(5)

and then (1) and (5) yield:

$$Sz^{\star}(G) - W(G) = PI_{v}(G) - n(n-1) + \sum_{\{x,y\}} \mu'_{x,y} + \frac{1}{4} \sum_{j=1}^{m} n_{0}(e_{j}) + \frac{n-1}{2} \sum_{x \in V(G)} m'_{x} - \frac{1}{2} \sum_{\{x,y\} \in \binom{V(G)}{2}} m'_{x,y}.$$
(6)

Since  $m_x = m - m'_x$ , Lemma 2.1 implies that

$$PI_{v}(G) = \sum_{x \in V(G)} (m - m'_{x}) = \sum_{e \in E(G)} (n - n_{0}(e)) = mn - \sum_{e \in E(G)} n_{0}(e).$$
(7)

By a double counting we can also state:

$$\sum_{\{x,y\}} m'_{x,y} = \sum_{e \in E(G)} \binom{n_0(e)}{2}.$$
(8)

Finally, from [12] we recall that

$$\sum_{\{x,y\}} \mu'_{x,y} \ge P(g) \,. \tag{9}$$

Inserting (7)-(9) into (6) and using the fact that  $\sum_{x \in V(G)} m'_x = \sum_{e \in E(G)} n_0(e)$ , we obtain

$$Sz^{\star}(G) - W(G) \geq mn - n(n-1) + P(g) + \frac{2n-5}{4} \sum_{e \in E(G)} n_0(e) - \frac{1}{2} \sum_{e \in E(G)} \binom{n_0(e)}{2},$$
  
done.  $\Box$ 

and we are done.

To characterize the equality cases in in Theorem 3.1, we need the following observation. Recall that a subgraph of a graph is called *isometric* if the distance between any two vertices of the subgraph is independent of whether it is computed in the subgraph or in the entire graph.

**Lemma 3.2** Let B be a block of a graph G and let x be a vertex of B. If B has at least three vertices, then x lies on some isometric cycle of G.

**Proof.** Since *B* is a block on at least three vertices, any two of its vertices lie on a common cycle. In particular, *x* lies on some cycle *C*. If *C* is isometric we are done. Otherwise, there exist vertices *u* and *v* of *C* and a *u*, *v*-path *P* which is internally disjoint with *C* and shorter than  $d_C(u, v)$ . Then the concatenation of *P* and the part of *C* from *u* via *x* to *v* is a cycle *C'* shorter than *C*. Since *C'* contains *x* we are done if *C'* is isometric. Otherwise, by repeating this procedure we obtain shorter cycles in each step, so we eventually must arrive at an isometric cycle containing *x*.

**Proposition 3.3** The equality in Theorem 3.1 holds if and only if G is an odd cycle, or g = 3 and  $\sum_{\{x,y\}} \mu'_{x,y} = 0$ .

**Proof.** Equations (6) and (9) from the proof of Theorem 3.1 imply that the equality holds if and only if  $\sum_{\{x,y\}} \mu'_{x,y} = P(g)$ . If g = 3 then P(g) = 0, hence the equality holds in this case if and only if  $\sum_{\{x,y\}} \mu'_{x,y} = 0$ .

Suppose next that g = 4. It was proved in [12] that for any isometric cycle C of G,  $\sum_{x,y\in C} \mu'_{x,y} = P(g)$  holds. Therefore, in order that the equality  $\sum_{\{x,y\}} \mu'_{x,y} = P(g)$  holds, G must contain a unique isometric cycle. Since any shortest cycle of a graph (as well as any shortest cycle of a block) is isometric, cf. [8, Proposition 3.3], it follows that G contains exactly one block B on more than two vertices. But then it follows from Lemma 3.2 that B must be isomorphic to a cycle, that is, to  $C_4$ . We conclude that G must be bipartite, hence there are no graphs with g = 4 that fulfil the equality.

Suppose finally that  $g \ge 5$ . Then we know from the proof of [12, Theorem 3.2] that  $\sum_{\{x,y\}} \mu'_{x,y} \ge (n-g)(g-3) + P(g)$ . Hence  $\sum_{\{x,y\}} \mu'_{x,y} = P(g)$  if and only if (n-g)(g-3) = 0 if any only if n = g if and only if  $G = C_n$ , where n is an odd integer at least 5.

It view of Proposition 3.3 it would be interesting to characterize the graphs with girth 3 and  $\sum_{\{x,y\}} \mu'_{x,y} = 0$ , in particular chordal graphs for which  $\sum_{x,y} \mu'_{x,y} = 0$  holds. For instance, block graphs belong to this family.

The estimate of Theorem 3.1 can be simplified as follows:

**Corollary 3.4** If G is a non-bipartite graph of order n, size m, and girth g, then

$$Sz^{\star}(G) - W(G) \ge n\left(m - \frac{3n}{4}\right) + P(g)$$

**Proof.** Using (8) and the equality  $\sum_{x \in V(G)} m'_x = \sum_{e \in E(G)} n_0(e)$ , the last two terms of the bound of Theorem 3.1 multiplied by 4 can be rewritten as

$$(2n-5)\sum_{x\in V(G)}m'_x-2\sum_{\{x,y\}}m'_{x,y}\,.$$

Since for any x and y,  $m'_x - m'_{x,y} \ge 0$ , it follows, having in mind Lemma 2.2, that

$$(2n-5)\sum_{x\in V(G)}m'_x - 2\sum_{\{x,y\}}m'_{x,y} \ge n(n-4)\,,$$

therefore the last two terms of the bound of Theorem 3.1 are bounded from below by n(n-4)/4 and the result follows.

Modifying the arguments from the proof of Theorem 3.1 we get the following improved lower bound for  $g \ge 5$ :

**Theorem 3.5** If G is a non-bipartite graph of order n, size m, and girth  $g \ge 5$ , then

$$Sz^{\star}(G) - W(G) \geq mn - n(n-1) + (n-g)(g-3) + P(g) + \frac{2n-5}{4} \sum_{e \in E(G)} n_0(e) - \frac{1}{2} \sum_{e \in E(G)} \binom{n_0(e)}{2}.$$

The equality holds if and only if G is composed of a 5-cycle and two trees rooted at two adjacent vertices of the cycle.

**Proof.** Suppose that G is a non-bipartite graph of girth  $g \ge 5$ . As already mentioned in the proof of Proposition 3.3,  $\sum_{\{x,y\}} \mu'_{x,y} \ge (n-g)(g-3) + P(g)$  holds in this case. Now, proceeding along the same line as in the proof of Theorem 3.1 (only replacing (9) with this stronger estimate) the lower bound follows.

The equality holds if and only if

$$\sum_{x,y} \mu'_{x,y} = (n-g)(g-3) + P(g).$$
(10)

Let  $C: v_1, v_2, \ldots, v_g, v_1$  be an arbitrary isometric cycle of G. Then by [12, Theorem 3.2],  $\sum_{\{x,y\}\in C} \mu'_{x,y} \ge P(g)$ . Moreover, if  $y \notin C$  and  $v_1$  is a vertex of C closest to y, then for any  $i \neq 1, 2, g$  we have  $\mu'_{v_i,y} \ge 1$ . Hence  $\sum_{\{v_i,y\}} \mu'_{v_i,y} \ge (n-g)(g-3)$ . Now, by (10) and an argument similar as in Proposition 3.3 we get that G is an (non-bipartite) unicycle graph. Hence, in order that the equality holds, the following must be fulfilled:

- (i)  $\mu'_{x,y} = 0$  holds for any  $x, y \notin C$ , and
- (ii)  $\mu'_{v_i,y} = 1$  as soon as  $i \neq 1, 2, g$  and  $y \notin C$ .

By [2, Lemma 2.4(2)] we know that  $\mu'_{x,y} \ge 1$  if  $d_C(v_i, v_j) \ge 2$ . Hence in order that (i) holds, G necessarily contains at most two non-trivial trees rooted at two adjacent vertices of C.

As for (ii), from the graph structure we find out  $\mu'_{v_1,v_i} = \mu'_{y,v_i}$ . Thus, if  $d(v_1, v_i) = 2$ with z a common neighbour of  $v_1$  and  $v_i$ , then, since C is an isometric odd cycle, for the edge e = uv that is antipodal to z on C we have d(z, u) = d(z, v). Therefore,  $v_1 \in N_u(e)$ and  $v_i \in N_v(e)$  (or the other way around), thus  $\mu'_{v_1,v_i} = 1$ . When  $d(v_1, v_i) = i \ge 3$ , the same reasoning yields  $\mu'_{v_1,v_i} \ge i - 1$ . Therefore, (ii) is satisfied when g = 5.  $\Box$ 

In parallel to Corollary 3.4 we can then state:

**Corollary 3.6** If G is a non-bipartite graph of order n, size m, and girth  $g \ge 5$ , then

$$Sz^{\star}(G) - W(G) \ge n\left(m - \frac{3n}{4}\right) + (n - g)(g - 3) + P(g)$$

If G be a connected graph with n vertices, m edges, p pendent vertices, and clique number  $\omega(\omega \ge 3)$  then in [3, Theorem 2.1] is proved  $PI_v(G) \ge 2m + (n-2)p + (n-\omega)(\omega-1)$ . Plug this inequality in (6) and by same process of Theorem 3.1 we get:

**Corollary 3.7** If G is a non-bipartite graph of order n, size m, girth g, clique number  $\omega(\omega \geq 3)$  and p pendent vertices, then

$$Sz^{\star}(G) - W(G) \geq 2m + (n-2)p + (n-\omega)(\omega-1) - n(n-1) + P(g) + \frac{2n-1}{4} \sum_{e \in E(G)} n_0(e) - \frac{1}{2} \sum_{e \in E(G)} {\binom{n_0(e)}{2}}.$$

## 4 Concluding remarks

Note that the bounds of Corollaries 3.4 and 3.6 extend the bound of Theorem 1.1 as soon as one of the conditions  $m \ge n + 1$  and  $g \ge 5$  holds. To conclude the paper we consider the remaining cases when m = n and g = 3, 4.

Hence let G be a graph with m = n, that is, a unicyclic graph. Suppose first that g = 4. Then G is bipartite and thus  $Sz(G) = Sz^{*}(G)$  holds. Therefore we can apply a better bound from [12].

Assume next that g = 3. Then the unique cycle of G is a triangle, say  $T = u_1 u_2 u_3$ . Let  $n_1, n_2$ , and  $n_3$  be the number of vertices of the three trees attached to the vertices of T, respectively, so that  $n = n_1 + n_2 + n_3$ . It is straightforward to verify that

- $\sum_{\{x,y\}\in V(G)} \mu'_{x,y} = 0,$
- $\sum_{e \in E(G)} n_0(e) = n$ , and
- $\sum_{e \in E(G)} {\binom{n_0(e)}{2}} = {\binom{n_1}{2}} + {\binom{n_2}{2}} + {\binom{n_3}{2}}.$

From (6) we can then deduce an exact formula for  $Sz^{\star}(G) - W(G)$ , in particular, the bound of Theorem 3.1 is sharp in this case.

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