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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 et al. (2014) proved that if G is a non-bipartite connected graph of order $n \geq 4$, then $Sz^\star(G) - W(G) \geq \left(n^2 + 4n - 6\right)/4$. 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.

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 topic, 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 as 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 $Sz^\star$ was proposed in [23]; it was named there the revised Wiener index. As expected, $Sz^\star(G) = Sz(G)$ holds for any bipartite graph G. The present name for $Sz^\star$ 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

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in [26,17], 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 $Sz(G) \geq W(G)$ holds for any connected graph [13], $Sz^\star(G) \geq W(G)$ holds as well. But how large the difference $Sz^\star(G) - W(G)$ 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 $n \geq 4$ vertices, then*

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

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, $Sz(G) = Sz^\star(G)$, 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

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

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 $m \geq n + 1$ and $g \geq 5$ 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 is 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 $PI_v(G) \geq n(n - 1)$. 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.