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On the difference between the Szeged and the Wiener index

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A B S T R A C T

We prove a conjecture of Nadjafi-Arani et al. on the difference between the Szeged and the Wiener index of a graph (Nadjafi-Aranifi et al., 2012). Namely, if G is a 2-connected non-complete graph on n vertices, then $Sz(G) - W(G) \geq 2n - 6$. Furthermore, the equality is obtained if and only if G is the complete graph K_{n-1} with an extra vertex attached to either 2 or $n-2$ vertices of K_{n-1}. We apply our method to strengthen some known results on the difference between the Szeged and the Wiener index of bipartite graphs, graphs of girth at least five, and the difference between the revised Szeged and the Wiener index. We also propose a stronger version of the aforementioned conjecture.

1. Introduction

Graph theoretic invariants of molecular graphs, which predict properties of the corresponding molecules, are known as topological indices or molecular descriptors. The oldest and most studied topological index is the Wiener index introduced in 1947 by Wiener [23], who observed that this invariant can be used for predicting the boiling points of paraffins. For a simple graph $G = (V, E)$, the Wiener index is defined as

$$W(G) = \sum_{\{a,b\} \subseteq V} d(a, b),$$

i.e., the sum of distances between all pairs of vertices. After 1947, the same quantity has been studied and referred to by mathematicians as the gross status [8], the distance of graphs [5], and the transmission [22]. A great deal of knowledge on the Wiener index is accumulated in research papers, e.g., [1,13,16,21], and surveys, e.g., [14,24], to mention just some recent ones.

Up to now, over 200 topological indices were introduced as potential molecular descriptors. Already in [23], Wiener introduced a related invariant now called the Wiener polarity index (see e.g., [15,17]), Another molecular descriptor motivated

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by the Wiener index is the Szeged index [6,9]; it was motivated by the original definition of Wiener index for trees. It is defined as

$$\mathrm{Sz}\,(G) = \sum_{ab\in E} n_{ab}(a) \cdot n_{ab}(b),$$

where $n_{ab}(a)$ is the number of vertices strictly closer to a than b, and analogously, $n_{ab}(b)$ is the number of vertices strictly closer to b. Note that $n_{ab}(a)$ and $n_{ab}(b)$ are always positive.

In this paper we consider possible values of the difference

$$\eta(G) = \mathrm{Sz}\,(G) - W(G)$$

between the Szeged and the Wiener index of a graph G. Klavžar et al. [12] proved that the inequality $\eta(G) \geq 0$ holds for every connected graph G. Moreover, Dobrynin and Gutman [4] showed that the equality is achieved if and only if G is a *block graph*, i.e., a graph in which every block (maximal 2-connected subgraph) induces a clique. Nadjafi-Arani et al. [18,19] further investigated the properties of $\eta(G)$ and proved that for every positive integer k, with $k \notin \{1, 3\}$, there exists a graph G with $\eta(G) = k$. Additionally, they classified the graphs G for which $\eta(G) \in \{2, 4, 5\}$ and asked about a general classification; namely, can we characterize all graphs with a given value of $\eta(G)$? They proposed the following conjecture.

Conjecture 1. [19] *Let G be a connected graph and let $B_1, \ldots, B_k$ be all its non-complete blocks of respective orders $n_1, \ldots, n_k$. Then*

$$\eta(G) \geq \sum_{i=1}^{k} (2n_i - 6).$$

In this paper, we prove the following statement which deals with 2-connected graphs.

Theorem 2. *If G is a 2-connected non-complete graph on n vertices, then*

$$\eta(G) \geq 2n - 6.$$

As a consequence of Theorem 2 we obtain that Conjecture 1 is true.

Corollary 3. *Let $B_1, \ldots, B_k$ be all the non-complete blocks of G with respective orders $n_1, \ldots, n_k$. Then*

$$\eta(G) \geq \sum_{i=1}^{k} (2n_i - 6).$$

In fact, we also characterize the graphs achieving equality in Theorem 2. For $n, t \in \mathbb{N}$ with $1 \leq t \leq n-1$, let K_n^t be the graph obtained from K_{n-1} by adding one new vertex adjacent to t of the $n-1$ old vertices. Observe that K_n^t is 2-connected and non-complete if $2 \leq t \leq n-2$. We prove the following stronger version of Theorem 2.

Theorem 4. *If G is a 2-connected non-complete graph on n vertices that is not isomorphic to K_n^2 or K_n^{n-2}, then*

$$\eta(G) \geq 2n - 5.$$

While $\eta(K_n) = 0$, and $\eta(K_n^2) = \eta(K_n^{n-2}) = 2n - 6$ (see Lemma 11 for the proof), there seems to be only a finite number of graphs G with $\eta(G) < 2n$; in particular, using a computer, we found such graphs of order at most 9, but none on 10 vertices. We therefore propose the following conjecture.

Conjecture 5. *Let G be a 2-connected graph of order $n \geq 10$ not isomorphic to K_n, K_n^2, or K_n^{n-2}. Then*

$$\eta(G) \geq 2n.$$

In Section 2, we derive Corollary 3 from Theorem 2. We present the proofs of Theorems 2 and 4 in Section 4, after introducing four technical lemmas in Section 3. In Section 5, we apply our method in order to obtain stronger versions of other results related to the difference between the Szeged and the Wiener index of a graph and, as corollaries, we present alternative proofs of the existing results. Finally, in Section 6 we use our approach to prove results for the revised Szeged index.

2. Preliminaries

In the paper, we will use the following definitions and notation. The *distance* $d(a, b)$ between two vertices a and b is the length of a shortest path between them. We say that an edge ab is *horizontal to a vertex* u if $d(u, a) = d(u, b)$. A cycle of length k is denoted by C_k. For a vertex u of G, by $N(u)$ and $N[u]$ we denote the *open* and the *closed neighborhood* of u, respectively; hence $N[u] = N(u) \cup \{u\}$. By extension, we define the open neighborhood $N(S)$ of a set S to be $(\cup_{a \in S} N(a)) \setminus S$. By $N_i(u)$ we denote the set of vertices that are at distance i from u. Hence $N_0(u) = \{u\}$, $N_1(u) = N(u)$, etc. The *degree* of u in G is denoted by $d(u)$ and we always denote the *number of vertices* of G by n, i.e., $n = |V(G)|$. A vertex is *dominating* if it is adjacent to all other vertices of a graph. A *non-edge* in a graph G is a pair of non-adjacent vertices. A *block* is a maximal