ON A RELATION BETWEEN SZEGED AND WIENER INDICES OF BIPARTITE GRAPHS

LILY CHEN, XUELIANG LI,* MENGMENG LIU AND IVAN GUTMAN

ABSTRACT. Hansen et. al., using the AutoGraphiX software package, conjectured that the Szeged index $Sz(G)$ and the Wiener index $W(G)$ of a connected bipartite graph G with $n \geq 4$ vertices and $m \geq n$ edges, obeys the relation $Sz(G) - W(G) \geq 4n - 8$. Moreover, this bound would be the best possible. This paper offers a proof to this conjecture.

1. Introduction

All graphs considered in this paper are finite, undirected and simple. We refer the readers to [3] for terminology and notation. Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. For $u, v \in V(G)$, $d(u, v)$ denotes the *distance* between u and v. If the graph G is connected, then its *Wiener index* is defined as

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v) \ .$$

This topological index has been extensively studied in the mathematical literature; see, e.g., [4, 6, 9, 10]. Let $e = uv$ be an edge of G. Define three sets as follows:

$$\begin{aligned} N_u(e) &= \{w \in V(G) : d(u, w) < d(v, w)\} \\ N_v(e) &= \{w \in V(G) : d(v, w) < d(u, w)\} \\ N_0(e) &= \{w \in V(G) : d(u, w) = d(v, w)\} \ . \end{aligned}$$

Thus, $\{N_u(e), N_v(e), N_0(e)\}$ is a partition of the vertex set of G with regard to $e \in E(G)$. The number of elements of $N_u(e)$, $N_v(e)$, and $N_0(e)$ will be denoted by $n_u(e)$, $n_v(e)$,

Supported by the "973" program and NSFC.
MSC (2000): Primary: 05C12; Secondary: 05C90.
Keywords: Distance (in graph), Wiener index, Szeged index.
Received: 11 January 2013, Accepted:
*Corresponding author.

and $n_0(e)$, respectively. Evidently, if n is the number of vertices of the graph G, then $n_u(e) + n_v(e) + n_0(e) = n$.

If G is bipartite, then the equality $n_0(e) = 0$ holds for all $e \in E(G)$. Therefore, for any edge e of a a bipartite graph, $n_u(e) + n_v(e) = n$.

A long time known property of the Wiener index is the formula [4, 11, 20]:

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

which is applicable for trees. Motivated by the above formula, one of the present authors [7] introduced a graph invariant, named as the *Szeged index*, defined by

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

where G is any graph, not necessarily connected. Evidently, the Szeged index is defined as a proper extension of the formula (1) for the Wiener index of trees.

Details of the theory of the Szeged index can be found in [8] and in the recent papers [1, 2, 5, 13, 13–18, 21].

In [12] Hansen et. al. used the AutoGraphiX software package and made the following conjecture:

Conjecture 1. *Let G be a connected bipartite graph with $n \geq 4$ vertices and $m \geq n$ edges. Then*

$$Sz(G) - W(G) \geq 4n - 8 \ .$$

Moreover the bound is best possible as shown by the graph composed of a cycle C_4 on 4 vertices and a tree T on $n-3$ vertices sharing a single vertex.

This paper offers a confirmative proof to this conjecture.

2. Main results

In [19], another expression for the Szeged index was put forward, namely

$$Sz(G) = \sum_{e=uv \in E(G)} n_u(e)\, n_v(e) = \sum_{e=uv \in E(G)} \sum_{\{x,y\} \subseteq V(G)} \mu_{x,y}(e) \tag{2}$$

where $\mu_{x,y}(e)$, interpreted as the contribution of the vertex pair x and y to the product $n_u(e)\, n_v(e)$, is defined as:

$$\mu_{x,y}(e) = \begin{cases} 1 & \text{if} \begin{cases} d(x,u) < d(x,v) \text{ and } d(y,v) < d(y,u) \\ \text{or} \\ d(x,v) < d(x,u) \text{ and } d(y,u) < d(y,v) \end{cases} \\ & \\ 0 & \text{otherwise.} \end{cases}$$

We first show that for a 2-connected bipartite graph Conjecture 1 is true.

Lemma 1. *Let G be a 2-connected bipartite graph of order $n \geq 4$. Then*

$$Sz(G) - W(G) \geq 4n - 8$$

with equality if and only if $G = C_4$.

Proof. From Eq. (2), we know that

$$\begin{aligned} Sz(G) - W(G) &= \sum_{\{x,y\} \subseteq V(G)} \sum_{e \in E(G)} \mu_{x,y}(e) - \sum_{\{x,y\} \subseteq V(G)} d(x,y) \\ &= \sum_{\{x,y\} \subseteq V(G)} \left[\sum_{e \in E(G)} \mu_{x,y}(e) - d(x,y) \right] . \end{aligned}$$

Claim: For every pair $\{x, y\} \subseteq V(G)$, we have

$$\sum_{e \in E(G)} \mu_{x,y}(e) - d(x,y) \geq 1 .$$

In fact, if $xy \in E(G)$, that is $d(x, y) = 1$, then we can find a shortest cycle C containing x and y since G is 2-connected. Then, $G[C]$ has no chord. Since G is bipartite, the length of C is even. There is an edge e' which is the antipodal edge of $e = xy$ in C. It is easy to check that $\mu_{x,y}(e') = \mu_{x,y}(e) = 1$. So the claim is true.

If $d(x, y) \geq 2$, let P_1 be a shortest path from x to y and P_2 be a second-shortest path from x to y, that is, $P_2 \neq P_1$ and $|P_2| = \min\{|P|| P \text{ is a path from } x \text{ to } y \text{ and } P \neq P_1\}$. Since G is 2-connected, P_2 always exists. If there is more than one path satisfying the condition, we choose P_2 as a one having the greatest number of common vertices with P_1 .

If $E(P_1) \bigcap E(P_2) = \emptyset$, let $P_1 \bigcup P_2 = C$, and then $|E(P_2)| \geq |E(P_1)|$ and all the antipodal edges of P_1 in C make $\mu_{x,y}(e) = 1$. We also know that $\mu_{x,y}(e) = 1$ for all $e \in E(P_1)$. Hence, $\sum_{e \in E(G)} \mu_{x,y}(e) - d(x,y) \geq d(x,y) > 1$.

If $E(P_1) \bigcap E(P_2) \neq \emptyset$, then $P_1 \triangle P_2 = C$, where C is a cycle. Let $P'_i = P_i \bigcap C = x' P_i y'$. It is easy to see that $|E(P'_2)| \geq |E(P'_1)|$, and the shortest path from x (or y) to the vertex v in P'_2 is xP_2x' (or yP_2y') together with the shortest path from x' (or y') to v in C. So, all the antipodal edges of P'_1 in C make $\mu_{x,y}(e) = 1$. We also know that $\mu_{x,y}(e) = 1$ for all $e \in E(P_1)$. Hence, $\sum_{e \in E(G)} \mu_{x,y}(e) = |E(P_1)| + d(x', y') \geq d(x, y) + 1$, which proves the claim.

Now, let $C = v_1v_2\dots v_pv_1$ be a shortest cycle in G, where p is even and $p \geq 4$. Actually, for every $e \in E(C)$ we have that $\mu_{v_i,v_{p/2+i}}(e) = 1$ for $i = 1, 2, \dots, \frac{p}{2}$. Then $\sum\limits_{e\in E(G)} \mu_{v_i,v_{p/2+i}}(e) = |C| = p$, that is, $\sum\limits_{e\in E(G)} \mu_{v_i,v_{p/2+i}}(e) - d(v_i, v_{p/2+i}) = p/2 \geq 2$. Combining this with the claim, we have that

$$Sz(G) - W(G) \geq \binom{n}{2} + \frac{p}{2}\left(\frac{p}{2} - 1\right) \geq \binom{n}{2} + 2 \geq 4n - 8\ .$$

The last two equalities hold if and only if $p = 4$, $n = 4$ or 5. If $n = 4, p = 4$, then $G \cong C_4$. If $n = 5, p = 4$, then $G \cong K_{2,3}$, and in this case we can easily calculate that $Sz(G) - W(G) > 12$. Thus, the equality holds if and only if $G \cong C_4$.

□

We now complete the proof of Conjecture 1 in the general case.

Theorem 2. *Let G be a connected bipartite graph with $n \geq 4$ vertices and $m \geq n$ edges. Then*

$$Sz(G) - W(G) \geq 4n - 8\ .$$

Equality holds if and only if G is composed of a cycle C_4 on 4 vertices and a tree T on $n - 3$ vertices sharing a single vertex.

Proof. We have proved that the conclusion is true for a 2-connected bipartite graph. Now suppose that G is a connected bipartite graph with blocks $B_1, B_2, \dots, B_k$, where $k \geq 2$. Let $|B_i| = n_i$. Then, $n_1 + n_2 + \dots + n_k = n + k - 1$. Since $m \geq n$ and G is bipartite, there exists at least one block, say B_1, such that $n_1 \geq 4$. Consider a pair $\{x, y\} \subseteq V$. We have the following four cases:

Case 1: $x, y \in B_i$, and $n_i \geq 4$. Then for every $e \in B_j$, $j \neq i$ we have $\mu_{x,y}(e) = 0$, which combined with Lemma 1 yields

$$\sum_{\{x,y\}\subseteq B_i} \left[\sum_{e\in E(G)} \mu_{x,y}(e) - d(x, y)\right] = \sum_{\{x,y\}\subseteq B_i} \left[\sum_{e\in E(B_i)} \mu_{x,y}(e) - d(x, y)\right] \geq 4n_i - 8\ .$$

Case 2: $x, y \in B_i$, and $n_i = 2$. In this case,

$$\sum_{\{x,y\}\subseteq B_i} \left[\sum_{e\in E(G)} \mu_{x,y}(e) - d(x, y)\right] = 0 = 4n_i - 8\ .$$

Case 3: $x \in B_1$, $y \in B_i$, $i \neq 1$. Let P be a shortest path from x to y, and let w_1, w_i be the cut vertices in B_1 and B_i , such that every path from a vertex in B_1 to B_i must go through w_1, w_i . By the proof of Lemma 1, we can find an edge $e' \in E(B_1) \backslash E(P)$, such that $\mu_{x,w_1}(e') = 1$. Because every path from a vertex in B_1 to y must go through w_1, we have $\mu_{x,y}(e') = 1$. We also know that $\mu_{x,y}(e) = 1$ for all $e \in E(P)$. Hence, $\sum\limits_{e \in E(G)} \mu_{x,y}(e) - d(x,y) \geq 1$.

We are now in the position to show that for all $y \in B_i \backslash \{w_i\}$, we can find a vertex $z \in B_1 \backslash \{w_1\}$ such that $\sum\limits_{e \in E(G)} \mu_{z,y}(e) - d(z,y) \geq 2$. Since B_1 is 2-connected with $n_1 \geq 4$, there is a cycle containing w_1. Let C be a shortest cycle containing w_1, say $C = v_1 v_2 \ldots v_p v_1$, where $v_1 = w_1$ and p is even. Set $z = v_{p/2+1}$. By the proof of Lemma 1, we have that $\sum\limits_{e \in E(B_1)} \mu_{z,w_1}(e) - d(z,w_1) \geq p/2 \geq 2$. It follows that there are two edges e', e'', that are not in the shortest path from z to w_1 , such that $\mu_{z,w_1}(e') = 1$ and $\mu_{z,w_1}(e'') = 1$. Thus, $\mu_{z,y}(e') = 1$ and $\mu_{z,y}(e'') = 1$. Hence, $\sum\limits_{e \in E(G)} \mu_{z,y}(e) - d(z,y) \geq 2$.

If we fix B_i , we obtain that

$$\sum_{\substack{x \in B_1 \backslash \{w_1\} \\ y \in B_i \backslash \{w_i\}}} \left[\sum_{e \in E(G)} \mu_{x,y}(e) - d(x,y) \right] \geq (n_1 - 1)(n_i - 1) + (n_i - 1) = n_1(n_i - 1) \ .$$

Case 4: $x \in B_i$, $y \in B_j$, $i \geq 2, j \geq 2, i \neq j$. Let P be a shortest path between x and y. If P passes through a block B_ℓ with $n_\ell \geq 4$, and $|B_\ell \bigcap P| \geq 2$, then we have that $\sum\limits_{e \in E(G)} \mu_{x,y}(e) - d(x,y) \geq 1$. Otherwise, $\sum\limits_{e \in E(G)} \mu_{x,y}(e) - d(x,y) \geq 0$. So,

$$\sum_{\substack{x \in B_i \backslash \{w_i\} \\ y \in B_j \backslash \{w_j\}}} \left[\sum_{e \in E(G)} \mu_{x,y}(e) - d(x,y)) \right] \geq 0 \ .$$

Equality holds if and only if P passes through a block B_ℓ with $n_\ell = 2$ or $n_\ell \geq 4$, and $|B_\ell \bigcap P| = 1$.

From the above four cases it follows that

$$Sz(G) - W(G) = \sum_{\{x,y\} \subseteq V(G)} \sum_{e \in E(G)} \mu_{x,y}(e) - \sum_{\{x,y\} \subseteq V(G)} d(x,y)$$

$$= \sum_{\{x,y\} \subseteq V(G)} \left[\sum_{e \in E(G)} \mu_{x,y}(e) - d(x,y) \right]$$

$$
\begin{aligned}
&= \sum_{i=1}^{k}\sum_{\{x,y\}\subseteq B_i}\left[\sum_{e\in E(G)}\mu_{x,y}(e)-d(x,y)\right]+\sum_{j=2}^{k}\sum_{\substack{x\in B_1\setminus\{w_1\}\\ y\in B_j\setminus\{w_j\}}}\left[\sum_{e\in E(G)}\mu_{x,y}(e)-d(x,y)\right]\\
&+ \frac{1}{2}\sum_{\substack{i\neq j\\ i\neq 1,j\neq 1}}\sum_{\substack{x\in B_i\setminus\{w_i\}\\ y\in B_j\setminus\{w_j\}}}\left[\sum_{e\in E(G)}\mu_{x,y}(e)-d(x,y)\right]\geq \sum_{i=1}^{k}(4n_i-8)+n_1\sum_{j=2}^{k}(n_j-1)\\
&= 4(n+k-1)-8k+n_1(n-n_1)=4n-4k-4+n_1(n-n_1)\ .
\end{aligned}
$$

Since $n_1+n_2+\cdots+n_k=n+k-1$, $n_1\geq 4$, $n_i\geq 2$, for $2\leq i\leq k$, we have that $4\leq n_1\leq n-k+1$, and $2\leq k\leq n-3$.

If $k\geq 5$, then $n_1(n-n_1)\geq 4(n-4)$. Thus,

$$
4n-4k-4+n_1(n-n_1)\geq 8n-4k-20\geq 8n-4(n-3)-20=4n-8\ .
$$

Equality holds if and only if $n_1=4$, $n_2=n_3=\cdots=n_{n-3}=2$ i.e., if $B_2,B_3,\ldots,B_{n-3}$ form a tree T on $n-3$ vertices, that shares a single vertex with B_1 .

If $2\leq k\leq 4$, then $n_1(n-n_1)\geq(n-k+1)(k-1)$.

If $k=2$, then $4n-4k-4+(n-k+1)(k-1)=5n-13\geq 4n-8$. Equality holds if and only if $n=5$, G is a graph composed of a cycle on 4 vertices and a pendant edge.

If $k=3$, then $4n-4k-4+(n-k+1)(k-1)=6n-20\geq 4n-8$. Equality holds if and only if $n=6$, G is a graph composed of a cycle on 4 vertices and a tree on 3 vertices sharing a single vertex.

If $k=4$, then $4n-4k-4+(n-k+1)(k-1)=7n-29\geq 4n-8$. Equality holds if and only if $n=7$, G is a graph composed of a cycle on 4 vertices and a tree on 4 vertices sharing a single vertex.

By this, the proof of Theorem 2 is completed. □

Remark 3. *The method used in the proof of Theorem 2 is not applicable to non-bipartite graphs. This is because given a 2-connected non-bipartite graph G, for any two vertices $x,y\in V(G)$, if C is an odd cycle, where C is defined as in Lemma 1, we cannot get $\sum_{e\in E(G)}\mu_{x,y}(e)-d(x,y)\geq 1$. Hence, for non-bipartite graphs we do not have an auxiliary result like Lemma 1.*

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Lili Chen, Xueliang Li, Mengmeng Liu
Center for Combinatorics, LPMC-TJKLC, Nankai University, Tianjin 300071, China
Email: lily60612@126.com , lxl@nankai.edu.cn , liumm05@163.com

Ivan Gutman
Faculty of Science, University of Kragujevac, P. O. Box 60, 34000 Kragujevac, Serbia
Email: gutman@kg.ac.rs