Wiener index versus Szeged index in networks

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Abstract

Let (G, w) be a network, that is, a graph $G = (V(G), E(G))$ together with the weight function $w : E(G) \to \mathbb{R}^+$. The Szeged index $Sz(G, w)$ of the network (G, w) is introduced and proved that $Sz(G, w) \geq W(G, w)$ holds for any connected network where $W(G, w)$ is the Wiener index of (G, w). Moreover, equality holds if and only if (G, w) is a block network in which w is constant on each of its blocks. Analogous result holds for vertex-weighted graphs as well.

Key words: Wiener index, Szeged index, network, block network

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1 Introduction

The Wiener index of a graph is the most famous and one of the most studied topological indices in mathematical chemistry. It was introduced back in 1947 but is nevertheless still a very active research topic, cf. [14, 15, 17, 18, 19].

The Szeged index of a graph was introduced in [8] and has received a lot of attention immediately after its introduction, cf. [4]. After that, a period of not so intensive research followed, but in the last years we are faced with a big revival of the interest for this index. Let us mention only a couple of recent developments. A conjecture from [10] led to a proof that the graphs G for which the Szeged index equals $\frac{|E(G)|\cdot|V(G)|^2}{4}$ are precisely connected, bipartite, distance-balanced graphs. (See [7] for distance-balanced graphs.) This result was independently obtained in [1] and in [6]. Pisanski and Randić [16] proposed to use the Szeged index (combined with the revised Szeged index) as a measure of bipartivity of a graph, see also [20]. For more recent results on the Szeged index we refer to [2, 5, 9, 14].

A *network* (G,w) is a graph $G=(V(G),E(G))$ together with the weight function $w:E(G)\to\mathbb{R}^+$. In this paper we consider the Wiener index and the Szeged index on networks (alias edge-weighted graphs). This seems to be a very natural framework, the weight of an edge could, for instance, measure the Euclidean distance between atoms in a molecular graph. However, this line of research seems not to be (widely) studied earlier, in particular, as far as we know, the *Szeged index of a network* (G,w), that we define as

$$Sz(G,w)=\sum_{e=uv} w(e)n_u(e)n_v(e)\,,$$

has not yet been defined on networks. (See below for the definition of $n_u(e)$.) In this paper we compare the Szeged index of a network (G,w) with its Wiener index $W(G,w)$ and prove the following:

Theorem 1 *Let* (G,w) *be a connected network. Then*

$$Sz(G,w)\geq W(G,w)\,.$$

Moreover, equality holds if and only if (G,w) *is a block network in which* w *is constant on each of its blocks.*

In the special case of graphs (that is, for networks in which $w\equiv 1$), the inequality part of Theorem 1 was proved in [13], see also [11], while the equality part was established in [3].

In the rest of the section we give definitions and concepts needed here. Then, is Section 2, a proof of Theorem 1 is given. In the concluding section we give some remarks on the theorem and observe that an analogous result holds for vertex-weighted graphs.

Let (G,w) be a connected network. The *distance* between vertices u and v of (G,w) is denoted by $d(u,v)$ and it is defined as the minimum sum of the weights of edges over all u,v-paths. The *Wiener index* $W(G,w)$ is the sum of the distances between all unordered pairs of vertices of (G,w). Every edge $e=uv\in E(G)$ induces the partition of the vertex set $V(G)$ of (G,w) into $V(G)=N_u(e)\bigcup N_v(e)\bigcup N_0(e)$ that

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

Set $n_u(e)=|N_u(e)|$ and $n_v(e)=|N_v(e)|$.

Finally, a *block* of a network is its maximal (with respect to inclusion) biconnected subnetwork. A network is called a *block network* if all of its blocks are complete.

2 Proof of Theorem 1

Let $|V(G)| = n$ and $|E(G)| = m$. Select shortest paths $P_1, P_2, \ldots, P_{\binom{n}{2}}$ in (G, w) such that for every pair of vertices $a, b \in V(G)$, $a \neq b$, there exists a unique shortest a, b-path in the list. Let $e_1, \ldots, e_m$ be an ordered list of edges of (G, w). Then define the path-edge matrix $D = [d_{ij}]$ of dimension $\binom{n}{2} \times m$ as follows:

$$d_{ij} = \begin{cases} w(e_j); & e_j \in E(P_i)\,, \\ 0; & e_j \notin E(P_i)\,. \end{cases}$$

It is clear that the summation of the entries of the i^{th} row of D is the length of the path P_i. Thus, the summation of all the entries of D is $W(G, w)$.

Suppose that P is a shortest a, b-path containing the edge $e_j = uv$. Traverse the path P from the source vertex a to the destination vertex b. If we traverse the vertex u before v, then $d(a, v) = d(a, u) + d(u, v)$. This implies that $a \in N_u(e_j)$ and $b \in N_v(e_j)$. It means that the number of non-zero entries in the j^{th} column of D is at most $n_u(e_j)n_v(e_j)$ and consequently, the summation of the entries of the j^{th} column of D is at most $w(e_j)n_u(e_j)n_v(e_j)$. It follows that $Sz(G, w) \geq W(G, w)$.

It also follows from the above double counting that $Sz(G, w) = W(G, w)$ if and only if for every $1 \leq j \leq m$, the summation of the j^{th} column is $w(e_j)n_u(e_j)n_v(e_j)$. This is in turn true if and only if the following conditions are fulfilled:

(1) Any two vertices of (G, w) are connected by a unique shortest path.

(2) For every edge $e = uv$ of (G, w) and every vertices $a \in N_u(e)$ and $b \in N_v(e)$, the shortest a, b-path contains e.

To complete the proof we will show that (G, w) is a block network and w is constant on each of its blocks if and only if conditions (1) and (2) hold. If (G, w) is a block network with w constant on blocks, (1) and (2) clearly holds. To prove the converse assume in the rest that (G, w) is an arbitrary network for which (1) and (2) hold.

Note first that the conditions imply that if uv is an edge, then the unique shortest u, v-path is the edge uv itself. It follows that if $e = uv$ and $f = ab$ are two edges of G such that $a \in N_u(e)$, then $b \notin N_v(e)$.

Let $e = uv$ and let $P_1 : u, t_1, t_2, \ldots, t_k, z$ be the shortest u, z-path, such that $t_i \in N_u(e), 1 \leq i \leq k$, and $z \in N_0(e)$. Let $P_2 : v, w_1, w_2, ..., w_r, y_{r+1}, \ldots, y_s = z$ be the shortest v, z-path, where $w_i \in N_v(e), 1 \leq i \leq r$, and $y_i \in N_0(e), r + 1 \leq i \leq s$. Set also $f = t_k z$ and $g = w_r y_{r+1}$. The situation is shown in Fig. 1.

Claim 1: The edges e, f and g form a triangle and $w(e) = w(f) = w(g)$.

Since P_1 is a shortest path, $u \in N_{t_k}(f)$. Therefore either $v \in N_{t_k}(f)$ or $v \in N_0(f)$. Suppose $v \in N_{t_k}(f)$. Then since $z \in N_z(f)$, the shortest v, z-path does not pass f which is not possible by condition (2). Therefore $v \in N_0(f)$. By a similar argument it follows that if $x \in N_v(e)$ then $x \in N_0(f)$. We conclude that $N_v(e) \subset N_0(f)$. Using a similar argument for the edge g, we also get $N_u(e) \subset N_0(g)$.

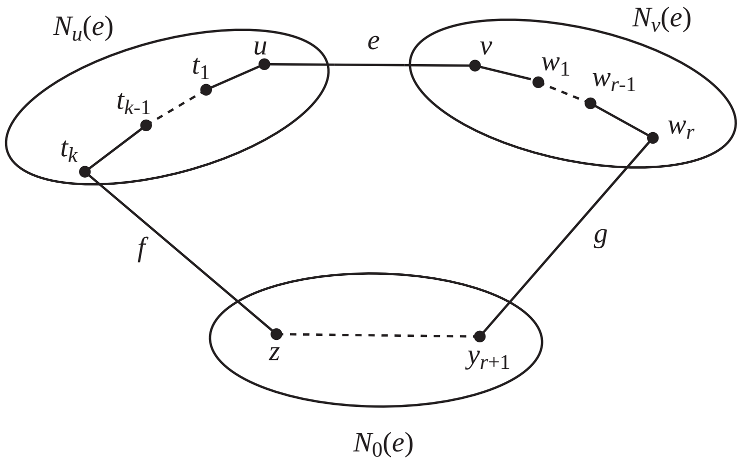

Figure 1: Situation from the proof

Since $w_r \in N_0(f)$ we have $d(t_k, w_r) = w(g) + d(y_s, y_{r+1})$. Moreover, as $t_k \in N_0(g)$ we have $d(t_k, w_r) = w(f) + d(y_s, y_{r+1})$, Therefore $w(f) = w(g)$.

We next prove that $w_r = v$ and $t_k = u$. Since $N_v(e) \subset N_0(f)$ and P_2 is a shortest path, the computation

$$\begin{aligned} d(t_k, w_{r-1}) &= d(z, w_{r-1}) \\ &= d(z, y_{r+1}) + w(g) + d(w_r, w_{r-1}) \\ &= d(t_k, w_r) + d(w_r, w_{r-1}) \\ &> d(t_k, w_{r-1}) \end{aligned}$$

gives a contradiction. Thus $v = w_r$. By a similar argument $t_k = u$. On the other hand, we have $w(f) = w(g)$. Then $d(u, z) = d(v, y_{r+1})$. But we also have $d(u, z) = d(v, z) = d(v, y_{r+1}) + d(z, y_{r+1}) = d(v, z) + d(z, y_{r+1})$. Hence $z = y_s = y_{r+1}$.

We conclude that the edges e, f, and g form a triangle in G and since $v \in N_0(f)$ we have $w(e) = w(f) = w(g)$.

Claim 2: There is no vertex $w \in N_v(e), w \neq v$, such that w is adjacent to some vertex in $N_0(e)$.

Suppose on the contrary that there is a vertex $w \neq v$ adjacent to $z' \in N_0(e)$. Set $\ell = wz'$. Since the shortest u, w-path passes e, we infer that $u \in N_0(\ell)$. So, if $w(e) = \alpha$ and $d(v, w) = \beta$ then $d(z', u) = \alpha + \beta$. Let $z \in N_0(e)$ be the last vertex of path $P : z', ..., z, u$. We proved before that z is adjacent to v and $w(uz) = w(vz) = \alpha$, hence $d(z, z') = \beta$. On the other hand, $v \in N_w(\ell)$. Indeed, if $v \notin N_w(\ell)$ then the shortest v, z'-path is of length at most β. On the other side, the distance between u and z' is $\alpha + \beta$, so $d(v, z') > \beta$, a contradiction. Similarly, $z \in N_{z'}(\ell)$. But the shortest v, z-path does not pass ℓ, a contradiction with condition (2).

Claim 3: If $z, z' \in N_0(e)$ are adjacent to u and v, then z and z' are adjacent.

Suppose z and z' are not adjacent. By Claim 1 we know that $w(uv) = w(uz) = w(vz) = w(uz') = w(vz') = \alpha$. The two distinct paths z, u, z' and z, v, z' have the same length 2α. By condition (1), there exists a (unique) shortest z, z'-path $L : z, z_1, \ldots, z_n = z'$ such that the length of L is less than 2α. By Claim 2, $V(L) \subseteq N_0(e)$. We now claim that $d(z, z') = \alpha$. For this sake we show that $z \in N_0(vz')$. If $z \in N_v(vz')$ (or $z \in N_{z'}(vz')$), then the shortest z, z'-path (z, v-path) does not pass the edge vz', a contradiction. Therefore $z \in N_0(vz')$ and hence $d(z, z') = d(v, z') = \alpha$. If $z_1 = z'$ nothing is to be proved. Suppose $z \neq z'$, then by a similar argument as above we see that $u, v \in N_0(z_{n-1}z')$. Thus $d(z_{n-1}, u) = d(z_{n-1}, v) = \alpha$. On the other hand, $z_{n-1} \in N_{z'}(vz')$ and $v \in N_v(vz')$, but the shortest v, z_{n-1}-path does not contain the edge vz', a contradiction. Therefore, z and z' are adjacent.

From Claims 1, 2, and 3 we conclude that (G, w) is a block network and w is constant on each of its blocks.

3 Concluding remarks

Consider the network (K_3, w), where $V(K_3) = \{x, y, z\}$ and $w(xy) = w(yz) = 2$ and $w(xz) = 3$. Note first that condition (1) from the previous section holds on (K_3, w). On the other hand, let $e = xy$, then $z \in N_y(e)$ and (clearly) $x \in N_x(e)$, but the shortest x, z-path does not contain the edge e. So condition (2) does not hold. And indeed, $W(K_3, w) = 7 \neq 11 = Sz(K_3, w)$.

Suppose now that (G, w_V) is a vertex-weighted graph, that is, the graph G together with a weight function $w_V : V(G) \to \mathbb{R}^+$. In this case, the Wiener index $W(G, w_V)$ of (G, w_V) is the sum, over all unordered pairs of vertices, of products of weights of the vertices and their distance [12], that is,

$$W(G, w_V) = \frac{1}{2} \sum_{u \neq v} w_V(u) w_V(v) d(u, v)\,.$$

Let $e = uv$ be an edge of (G, w_V), then define $n_u(e) = \sum_{t \in N_u(e)} w_V(t)$ and set

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

Theorem 2 *Let (G, w_V) be a vertex-weighted graph. Then $Sz(G, w_V) = W(G, w_V)$ if and only if every block of (G, w_V) is a complete.*

Proof. Similarly as in the beginning of the proof of Theorem 1, select shortest paths $P_1, P_2, \ldots, P_{\binom{n}{2}}$ in (G, w_V). Let P_i from this list be a shortest a, b-path, then we will denote it $P_i(a, b)$. Define the path-edge matrix $E = [e_{ij}]$ as follow:

$$e_{ij} = \begin{cases} w_V(a) w_V(b); & e_j \in E(P_i(a, b))\,, \\ 0 & e_j \notin E(P_i(a, b))\,. \end{cases}$$

It is clear that the summation of the entries of the i^{th} row of E is $w_V(a) w_V(b) d(a, b)$. Thus, the summation of the entries of E is $W(G, w_V)$. It is easy to see that the summation of the entries of the j^{th} column of E is at most $n_u(e_j)n_v(e_j)$, where $e_j = uv$. It follows that $Sz(G, w_V) \geq W(G, w_V)$. So, equality holds if and only if the conditions (1) and (2) are fulfilled. Clearly, these conditions are equivalent to the condition that every block of (G, w_V) is complete. $\square$

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