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.

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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

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

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

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

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 $(\cup_{a \in S} N(a)) \backslash S$. 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
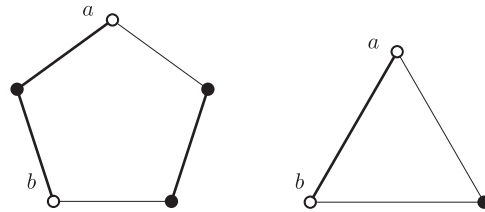
Fig. 1. Cycles C_5 and C_3 with good edges for the pair a and b depicted in bold.

subgraph without a cut-vertex. Note that a block is either a 2-connected subgraph, a single edge or an isolated vertex, and every graph has a unique decomposition into blocks. If $B \subseteq V(G)$, then $G[B]$ denotes the subgraph of G induced by B.

For an unordered pair of vertices a and b, an edge $e = uv$ is *good* for $\{a, b\}$ if $d(a, u) < d(a, v)$ and $d(b, v) < d(b, u)$. Let $g(a, b)$ be the *number of good edges* for $\{a, b\}$. Note that every edge on a shortest path between a and b is a good edge for $\{a, b\}$, which gives $g(a, b) \geq d(a, b)$ (Fig. 1).

The concept of good edges has been introduced by Simić et al. [20] and used for an alternative definition of the Szeged index. Observe that an edge uv is good for exactly $n_{uv}(u) \cdot n_{uv}(v)$ pairs of vertices. Therefore,

$$Sz(G) = \sum_{uv \in E} n_{uv}(u) \cdot n_{uv}(v) = \sum_{\{a,b\} \subseteq V} g(a, b). \tag{1}$$

Consequently, we obtain the following statement.

Proposition 6. *Let G be a graph. Then*

$$\eta(G) = \sum_{\{a,b\} \subseteq V} \big(g(a, b) - d(a, b)\big).$$

To simplify the notation, we write

$$\eta(a, b) = g(a, b) - d(a, b).$$

Note that $g(a, a) = d(a, a) = 0$. Since $g(a, b) \geq d(a, b)$ for every pair a, b, we easily obtain the known fact that $Sz(G) \geq W(G)$.

Next, we define the *contribution* $c_G(a)$ of a vertex a in a graph G as

$$c_G(a) = \sum_{b \in V} \eta(a, b) = \sum_{b \in V} \big(g(a, b) - d(a, b)\big). \tag{2}$$

When there is no ambiguity from the context, we write $c(a)$ instead of $c_G(a)$. Therefore,

$$\eta(G) = \frac{1}{2} \sum_{a \in V} c(a). \tag{3}$$

Now we are ready to prove Corollary 3 using Theorem 2.

Proof of Corollary 3. Note first that for any a, b from B_i it holds $g_{B_i}(a, b) = g_G(a, b)$ and $d_{B_i}(a, b) = d_G(a, b)$. By Theorem 2, we have

$$\eta(B_i) = \sum_{\{a,b\} \subseteq V(B_i)} \eta(a, b) = \sum_{\{a,b\} \subseteq V(B_i)} \big(g(a, b) - d(a, b)\big) \geq 2n_i - 6,$$

for every i, $1 \leq i \leq k$. Since $g(a, b) \geq d(a, b)$ for every $\{a, b\} \subseteq V$, we conclude that

$$\eta(G) = \sum_{\{a,b\} \subseteq V} \big(g(a, b) - d(a, b)\big) \geq \sum_{i=1}^{k} (2n_i - 6).$$

$\square$

3. Auxiliary results

In this section, we prove four technical lemmas which will be used in the next sections to prove our theorems.

We first show that some vertices allow for an inductive argument.

Lemma 7. *Let G be a 2-connected graph. If G contains a vertex u such that $G - u$ is 2-connected, not complete, and there exists a vertex v such that $N[u] \subseteq N[v]$, then $\eta(G) - \eta(G - u) \geq 2$.*

Proof. Let $G = (V, E)$ be a graph satisfying the assumptions, and let $G^* = G - u$. Since G^* is not complete, neither is the graph G. Since $N[u] \subseteq N[v]$, we have that $d_{G^*}(a, b) = d_G(a, b)$ for any two vertices distinct from u. Hence,

$$W(G) = W(G^*) + \sum_{a \in V \setminus \{u\}} d(u, a).$$

Let q be the number of couples $(\{a, b\}, w)$ such that a, b are vertices of G^* and w is a neighbor of u such that the edge uw is good for $\{a, b\}$. Similarly as above, one can easily verify that

$$\mathrm{Sz}\,(G) = \mathrm{Sz}\,(G^*) + \sum_{a \in V \setminus \{u\}} g(u, a) + q\,.$$

Therefore,

$$\eta(G) - \eta(G^*) = \sum_{a \in V \setminus \{u\}} \big(g(u, a) - d(u, a)\big) + q, \tag{4}$$

and it suffices to prove that the right-hand side of (4) is at least 2. In order to do so, we consider the following contributions:

- (C1) *q is at least twice the number of non-edges in $N(u)$. Indeed, for any two non-adjacent neighbors w_1, w_2 of u, the edges uw_1 and uw_2 are both good for $\{w_1, w_2\}$, and so each of the couples $(\{w_1, w_2\}, w_1)$ and $(\{w_1, w_2\}, w_2)$ contributes 1 to q.*
- (C2) *For every vertex $a \notin N[u]$, we have $g(u, a) - d(u, a) \geq 2(p_a - 1)$, where p_a is the number of neighbors w of a with $d(u, w) < d(u, a)$. This follows from the fact that both edges, aw and ww' (w' being a neighbor of w with $d(u, w') < d(u, w)$), are good for the pair $\{u, a\}$, for every w.*
- (C3) *For every edge ab horizontal to u, and for every neighbor x of a, with $d(u, x) < d(u, a)$, such that x is not adjacent to b, the edge ax is good for $\{u, b\}$, i.e., it contributes an extra 1 to $g(u, b) - d(u, b)$.*

If u is dominating, then, since G is not a complete graph, there is a missing edge in $N(u)$ and $q \geq 2$ by (C1).

Assume now that u is not dominating. We show that $\sum_{a \in V \setminus \{u\}} \big(g(u, a) - d(u, a)\big) \geq 2$. If there is exactly one vertex that does not belong to $N[u]$, then it must have at least two neighbors in $N(u)$ since G is 2-connected, and the conclusion follows from (C2).

From now on, we assume that there are at least two vertices that do not belong to $N[u]$. Since G is 2-connected, there are at least two vertices in $N(N[u])$. If there is a vertex having at least two neighbors in $N(u)$, we have $\sum_{a \in V \setminus \{u\}} \big(g(u, a) - d(u, a)\big) \geq 2$, by (C2). So we may assume that any vertex $a \in N(N[u])$ has exactly one neighbor x in $N(u)$. Since G is 2-connected, the graph $G - x$ is connected. Let P be a shortest path between a and u in $G - x$. Note that P contains:

- a vertex b having two neighbors y_1 and y_2 with $d(u, y_1) = d(u, y_2) < d(u, b)$; or
- an edge $b_1 b_2$ horizontal to u with the property that for the other neighbors, z_1 and z_2, of b_1 and b_2 in P, respectively, it holds $d(u, z_i) < d(u, b_i)$, $i \in \{1, 2\}$, and $b_1 z_2, b_2 z_1 \notin E$.

By (C2) and (C3), we infer that $\sum_{a \in V \setminus \{u\}} (g(u, a) - d(u, a)) \geq 2$ in either case, and so we conclude that $\eta(G) - \eta(G^*) \geq 2$. $\square$

In the forthcoming lemma, we characterize the graphs G for which the difference $\eta(G) - \eta(G - u)$ attains 2.

Lemma 8. *Let G be a 2-connected graph of order n containing a vertex u such that $G - u$ is 2-connected, not complete, and there exists a vertex v such that $N[u] \subseteq N[v]$. If $\eta(G) - \eta(G - u) = 2$ and $G - u$ is isomorphic to K_{n-1}^2 or K_{n-1}^{n-3}, then G is isomorphic to K_n^2 or K_n^{n-2}.*

Proof. Note that $n \geq 5$, since $G - u$ is 2-connected and non-complete. Let $G^* = G - u$ and let α be the number of ordered triples (x, y, z) such that y is adjacent to both x and z and $d(u, x) < d(u, y)$, and either

(a) $d(u, z) < d(u, y)$; or
(b) the edge yz is horizontal to u and x is not adjacent to z.

From the proof of Lemma 7, we know that either u is dominating and, by (C1), there is precisely one edge missing in $N(u)$, or u is not dominating and, by (C2) or (C3), $\alpha \leq 2$. In the first case we immediately obtain that G^* is isomorphic to K_{n-1}^{n-3}, and so G is isomorphic to K_n^{n-2}. Therefore, we may assume that u is not dominating, $N(u)$ induces a clique and $\alpha \leq 2$.

In what follows, we show that $|N(N[u])| = 1$. Since G^* is isomorphic to K_{n-1}^{n-3} or K_{n-1}^2, it contains at least two dominating vertices. Note that every dominating vertex of G^* is in $N(u)$ or $N(N[u])$.

Suppose first there are two dominating vertices of G^* in $N(u)$, say w_1 and w_2. Then, for every $a \in N(N[u])$ both (w_1, a, w_2) and (w_2, a, w_1) contribute 1 to α and hence $|N(N[u])| \leq 1$.

Suppose now there is a dominating vertex w in $N(N[u])$. Then, due to the 2-connectivity of G, w has at least two neighbors, say a_1 and a_2, in $N(u)$ and consequently both (a_1, w, a_2) and (a_2, w, a_1) contribute 1 to α. If there is a vertex $z \neq w$ with $z \in N(N[u])$, then $wz \in E(G^*)$ as w is dominating in G^*, and either $a_i z \notin E(G^*)$ in which case (a_i, w, z) contributes 1 to α, or $a_1 z, a_2 z \in E(G^*)$ in which case (a_1, z, a_2) contributes 1 to α. Consequently, $|N(N[u])| \leq 1$ also in this case.

So, in both cases we have $|N(N[u])| \leq 1$ and since u is not dominating in G, we conclude $|N(N[u])| = 1$. Denote by z the unique vertex of $N(N[u])$. Since G is 2-connected and $\alpha \leq 2$, z has exactly two neighbors in $N(u)$, which forms a clique. Consequently, G^* is isomorphic to K_{n-1}^2 and G is isomorphic to K_n^2. $\square$

In the next lemma we also assume existence of two vertices, one of which dominates the other.

Lemma 9. *Let G be a 2-connected non-complete graph distinct from K_4^2. Suppose that for every pair of vertices u, v with $N[u] \subseteq N[v]$, $G - u$ is complete or not 2-connected, and at least one such a pair exists. Then for every two vertices u, v, where $N[u] \subseteq N[v]$, it holds that $G - u$ is not 2-connected and no block of $G - u$ is isomorphic to K_t, K_t^2 or K_t^{t-2} for any t.*

Proof. Suppose there is a pair u, v with $N[u] \subseteq N[v]$ and $G - u$ is complete. Then u is not dominating in G and $V = \{u\} \cup N(u) \cup N(N[u])$. If $N(N[u])$ contains at least two vertices w_1, w_2, then these vertices satisfy $N[w_1] = N[w_2]$, and $G - w_1$ is 2-connected but not complete, which contradicts assumptions of the lemma. So, let w be the unique vertex in $N(N[u])$. Let v_1, v_2 be two vertices in $N(u)$ (such vertices exist since G is 2-connected). We have $N[v_1] = N[v_2]$. If $N(u)$ is of size at least three, then $G - v_1$ is 2-connected but not complete, a contradiction. If $N(u)$ is of size two, then G is isomorphic to K_4^2, a contradiction.

By the above paragraph, we may assume that for every pair u, v where $N[u] \subseteq N[v]$, the graph $G - u$ is not 2-connected. Note that v is contained in every block of $G - u$ and is the only cut-vertex in $G - u$.

Next, suppose for a contradiction that there is a pair u, v with $N[u] \subseteq N[v]$ such that a block C of $G - u$ is isomorphic to K_t, K_t^2 or K_t^{t-2} for some t. Observe that each of K_t, K_t^2 and K_t^{t-2} has at least two dominating vertices since $t \geq 2$. Moreover, since G is 2-connected, there is a vertex $x \in N(u)$ distinct from v in C. We distinguish two cases:

Case 1. *The vertex v dominates C.* Then, every vertex $w \in V(C) \setminus \{v\}$ satisfies $N[w] \subseteq N[v]$, and so $G - w$ is not 2-connected. If $|V(C)| = 2$, i.e., if C is a trivial block consisting of a single edge, then x is the only vertex of C distinct from v and $d(x) = 2$ since $xv, xu \in E$. Since $G - x$ is not 2-connected, while G is, $G - x$ must be a single edge. Consequently G is isomorphic to K_3, a contradiction. Hence $|V(C)| \geq 3$.

Let $z \in V(C) \setminus \{v, x\}$. If C contains a dominating vertex w such that $w \notin \{v, z\}$, then $G - z$ is 2-connected, a contradiction. However since C is isomorphic to K_t, K_t^2 or K_t^{t-2}, it contains at least one dominating vertex w other than v. This means that C contains at most three vertices, and hence $|V(C)| = 3$. Since C has two dominating vertices, C is isomorphic to K_3, and consequently $G - z$ is 2-connected, a contradiction.

Case 2. *The vertex v does not dominate C.* Then C is not K_t. As mentioned above, there are at least two dominating vertices in C, and if C is distinct from K_4^2, then there are at least three dominating vertices in C since $C \neq K_4^2$.

First suppose that C has at least three dominating vertices w_1, w_2, w_3. If $w_1 u \notin E$, then $N[w_1] \subseteq N[w_2]$ and $G - w_1$ is 2-connected, a contradiction. On the other hand if $w_1 u \in E$, then $N[w_2] \subseteq N[w_1]$ and $G - w_2$ is 2-connected, a contradiction.

Thus, C has exactly two dominating vertices, say w_1 and w_2. Then C is isomorphic to K_4^2. Observe that $|V(C)| \geq 4$. If $w_1 u \in E$, then for every vertex z of C, $z \notin \{v, w_1, w_2\}$, we have $N[z] \subseteq N[w_1]$ and $G - z$ is 2-connected, a contradiction. Therefore $w_1 u, w_2 u \notin E$. Let z be the vertex of degree 2 in C. Then $z \notin \{w_1, w_2\}$, and since $N[u] \subseteq N[v]$, also $z \neq v$. If $zu \notin E$, then $N[z] \subseteq N[w_1]$ and $G - z$ is 2-connected, a contradiction. On the other hand if $zu \in E$, then $N[w_1] \subseteq N[w_2]$ and $G - w_1$ is 2-connected, a contradiction.

This completes the proof of the lemma. $\square$

We now describe how to deal with the case when there are no two vertices u, v with $N[u] \subseteq N[v]$.

Lemma 10. *Let G be a 2-connected non-complete graph distinct from C_5 with no two vertices u, v satisfying $N[u] \subseteq N[v]$. Then $c(u) \geq 4$ for every vertex u, and hence $\eta(G) \geq 2n$.*

Proof. Let G be a graph satisfying the assumptions of the lemma. Assume for a contradiction that there is a vertex a such that $c(a) \leq 3$. Consider a breadth-first-search tree of G rooted at a, with the levels $N_0, \ldots, N_p$, where p is the eccentricity of a. Then $N_i = N_i(a)$.

Observe first that $p \geq 2$. Indeed, if $p = 1$, then for every $x \in V \setminus \{a\}$, we have $N[x] \subseteq N[a]$. Therefore, G would contain only one vertex, namely the vertex a, which contradicts the 2-connectivity of G.

Note also that for every i, $1 \leq i \leq p - 1$, we have $|E(N_i, N_{i+1})| \geq |N_{i+1}|$, and since G is 2-connected, we have also $|N_i| \geq 2$. In what follows, for every $x \in V \setminus \{a\}$, we denote by $f(x)$ the number such that $x \in N_{f(x)}$. When the vertex x is clear from the context, we sometimes refer to the level $N_{f(x)-1}$ as the *previous level*.

We say that a vertex x has the property P_1 if it is adjacent to two vertices in the level $N_{f(x)-1}$. Moreover, if there is a pair of adjacent vertices x_1, x_2 in a same level each having precisely one neighbor y_1, y_2, respectively, in the previous level, and $y_1 \neq y_2$, then both these vertices have the property P_2.

In what follows we prove several claims about G.

Claim 1. *There is at most one vertex x with the property P_1. In the case when such a vertex x exists, it has exactly two neighbors in $N_{f(x)-1}$.*

Proof. Let x be a vertex distinct from a, and let $y_1, \ldots, y_\ell$ be the neighbors of x in $N_{f(x)-1}$. Suppose that $\ell \geq 2$ (this implies that $f(x) \geq 2$). For each $i \in \{1, \ldots, \ell\}$, let z_i be a neighbor of y_i in $N_{f(x)-2}$. Obviously, z_i's need not be distinct. Anyway,

similarly as ($C2$) in the proof of Lemma 7,

$$\eta(a, x) = g(a, x) - d(a, x) \geq 2 \cdot (\ell - 1),$$

since all the edges xy_i, y_iz_i are good for the pair $\{a, x\}$ and there is a shortest path between a and x containing at most two of these edges. Since $c(a) \leq 3$, no vertex of G has three neighbors in the previous level, and at most one has two neighbors in the previous level. This establishes the claim. $\square$

Claim 2. *There is at most one pair of vertices $\{x, y\}$ with the property P_2. If such a pair exists, then there is no vertex $z \in V \backslash \{x, y\}$ with the property P_1.*

Proof. Let x and y be a pair of adjacent vertices with the property P_2. Then, there exist two distinct vertices w, z in $N_{f(x)-1}$ such that x is adjacent to w and y is adjacent to z. We make no assumption about whether x is adjacent to z, but by Claim 1, we may assume that y is not adjacent to w. Therefore the edge wx is good for $\{a, y\}$. If x is not adjacent to z, then the edge yz is good for $\{a, x\}$, and if x is adjacent to z, then analogously as in Claim 1, there are two edges around z, which are good for $\{a, x\}$. Anyway, $g(a, x) - d(a, x) \geq 1$ and $g(a, y) - d(a, y) \geq 1$.

Now assume that we have two such pairs $\{x_1, y_1\}$ and $\{x_2, y_2\}$. If the two pairs are disjoint, then we have $\eta(a, u) \geq 1$ for each $u \in \{x_1, x_2, y_1, y_2\}$, which contradicts $c(a) \leq 3$. If they are not disjoint, then without loss of generality we may assume $x_1 = x_2$, in which case $y_1 \neq y_2$. From the previous analysis, we have $\eta(a, y_1) \geq 1$ and $\eta(a, y_2) \geq 1$. We claim that $g(a, x_1) - d(a, x_1) \geq 2$. Indeed, either x_1 has two neighbors in the previous level, or x_1 has exactly one neighbor in the previous level and for z_1 and z_2 being respective neighbors of y_1 and y_2 in the previous level, both y_1z_1 and y_2z_2 are good for $\{a, x_1\}$. Hence the first conclusion holds.

Finally, if there is a vertex $z \in V \backslash \{x, y\}$ with two neighbors in the previous level, then the conclusion follows as $\eta(a, z) \geq 2$, and hence $c(a) \geq 4$. This establishes the claim. $\square$

Claim 3. *In every connected component of $G[N_p]$ there is either a vertex with the property P_1 or a pair of adjacent vertices which have the property P_2.*

Proof. Let C be a connected component of $G[N_p]$. Suppose first that no vertex in C has P_1. Then, since G is 2-connected, every vertex of C has a neighbor in N_p. If there exists an edge $e = uv$ such that u, v are not both adjacent to the same unique neighbor of N_{p-1}, then u and v have property P_2 and we are done. Hence, the endvertices of each edge e of C are both adjacent to a unique vertex $x_e \in N_{p-1}$. But, since C is connected, all the x_e's coincide and thus a unique vertex $x \in N_{p-1}$ is adjacent to all the vertices in C. Since $p \geq 2$, x is a cut-vertex of G and so G is not 2-connected, a contradiction.

Now, suppose that there is a vertex x^* with P_1 and a pair of adjacent vertices x_1, x_2 with P_2 in C. By Claim 2, $x^* \in \{x_1, x_2\}$. Without loss of generality we may assume that $x^* = x_1$. Denote by y_1 and y_2 the two distinct neighbors of x_1 in N_{p-1}, and denote by y_3 the unique neighbor of x_2 in N_{p-1}. If $y_3 \notin \{y_1, y_2\}$, then x_1y_1, x_1y_2 are good for $\{a, x_2\}$ and x_1y_1, x_1y_2, x_2y_3 are good for $\{a, x_1\}$, which gives $g(a, x_2) - d(a, x_2) \geq 2$ and $g(a, x_1) - d(a, x_1) \geq 2$ and consequently $c(a) \geq 4$, a contradiction. Hence, $y_3 \in \{y_1, y_2\}$. By Claim 1, every neighbor of x_2 in N_p, other than x_1, is adjacent to a unique vertex of N_{p-1}. By Claim 2, this vertex must be y_3, meaning that $N[x_2] \subseteq N[y_3]$, which contradicts the assumption. $\square$

By the previous claims, the vertices with the properties P_1 or P_2 are only in N_p. Moreover, there is either one vertex with P_1 or a pair of adjacent vertices with P_2 and N_p has only one component. Next claim deals with vertices which have neither P_1 nor P_2.

Claim 4. *Let u be a vertex which has neither P_1 nor P_2. Then u has a neighbor in $N_{f(u)+1}$.*

Proof. By way of contradiction, assume that u has no neighbors in $N_{f(u)+1}$. Then $u \neq a$. Since u does not have P_1, it has a unique neighbor, say v, in $N_{f(u)-1}$. Since G is 2-connected, u must have a neighbor in $N_{f(u)}$. Let w be a neighbor of u in $N_{f(u)}$. If $vw \notin E$, then u and w have P_2, a contradiction. Hence, $vw \in E$. Consequently, $N[u] \subseteq N[v]$ contradicting the assumption. $\square$

By Claims 3 and 4, every vertex in N_p has either P_1 or P_2. We consider the two cases separately.

Case 1. *There is $x \in N_p$ with the property P_1.* By Claims 1 and 2, x is the only vertex in G with the properties P_1 or P_2. Hence, by Claims 3 and 4, we have $N_p = \{x\}$. Denote by y_1 and y_2 the two neighbors of x in N_{p-1}. If there is $y^* \in N_{p-1} \backslash \{y_1, y_2\}$, then it has neither P_1 nor P_2 by Claims 1 and 2, and so by Claim 4, y^* has a neighbor in $N_p = \{x\}$, a contradiction. Thus, $N_{p-1} = \{y_1, y_2\}$. Let z_i be a neighbor of y_i in N_{p-2}, $1 \leq i \leq 2$.

First, suppose that $z_1 \neq z_2$. Then $p \geq 3$. Let b_i be the unique neighbor of z_i in N_{p-3}, where $1 \leq i \leq 2$. Then all the edges b_1z_1, z_1y_1, y_1x, b_2z_2, z_2y_2, y_2x are good for $\{a, x\}$ which gives $\eta(a, x) \geq 3$. If $y_1y_2 \in E$, then we have $N[x] \subseteq N[y_1]$, which contradicts the assumption; thus we have $y_1y_2 \notin E$, which means that y_1x is good for $\{a, y_2\}$. Hence $g(a, y_2) - d(a, y_2) \geq 1$ and consequently $c(a) \geq 4$, a contradiction.

Thus, suppose that $z_1 = z_2$. If $|V| > 4$, then z_1 is a cut-vertex which contradicts the 2-connectivity of G. Hence, $|V| = 4$. Then G is either C_4 or C_4 with a chord, depending on whether y_1y_2 is or is not in E. However, if $y_1y_2 \in E$ then $N[y_1] \subseteq N[y_2]$, while if G is C_4 then $c(a) = 4$ for every $a \in V(C_4)$; both these cases contradicting the assumptions.

Case 2. *There is a pair of adjacent vertices x_1, $x_2 \in N_p$ with the property P_2.* Similarly as above, $N_p = \{x_1, x_2\}$. By Claim 3, both x_1 and x_2 have a unique neighbor in N_{p-1}. Let y_i be the neighbor of x_i in N_{p-1}, where $1 \leq i \leq 2$. If $y_1 = y_2$, then y_1 is a cut-vertex which contradicts the 2-connectivity of G. Hence $y_1 \neq y_2$. By Claim 2, each y_i has a unique neighbor z_i in N_{p-2}. Analogously as in Case 1, we have $N_{p-1} = \{y_1, y_2\}$.

Suppose that $z_1 \neq z_2$. Then the edges $z_1 y_1$, $y_1 x_1$ are good for $\{a, x_2\}$ and $z_2 y_2$, $y_2 x_2$ are good for $\{a, x_1\}$ which gives $\eta(a, x_2) \geq 2$ and $\eta(a, x_1) \geq 2$ and consequently $c(a) \geq 4$, a contradiction.

Thus, suppose that $z_1 = z_2$. If $|V| > 5$ then z_1 is a cut-vertex which contradicts the 2-connectivity of G. Hence, $|V| = 5$. Then G is either C_5 or C_5 with a chord, depending on whether $y_1 y_2$ is or is not in E. Since in the case $y_1 y_2 \in E$ we have $N[z_1] \subseteq N[y_1]$, G is C_5. $\square$

4. Proof of Theorem 4

We start with a lemma about $\eta(K_n^2)$ and $\eta(K_n^{n-2})$.

Lemma 11. *We have $\eta(K_n^2) = \eta(K_n^{n-2}) = 2n - 6$.*

Proof. Let $G \in \{K_n^2, K_n^{n-2}\}$. Denote by u a vertex of smallest degree in G. Since the eccentricity of u is 2, we have $V(G) = N_0(u) \cup N_1(u) \cup N_2(u)$. Since both $G[N_0(u) \cup N_1(u)]$ and $G[N_1(u) \cup N_2(u)]$ are cliques, $\eta(x_1, x_2) > 0$ for $x_1, x_2 \in V(G)$ only if $u \in \{x_1, x_2\}$, say $u = x_1$, and the other vertex x_2 is in $N_2(u)$. In the case $G = K_n^2$, there are $n - 3$ vertices x_2 in $N_2(u)$ and for each of them $\eta(u, x_2) = 2$. On the other hand if $G = K_n^{n-2}$, there is a unique vertex x_2 in $N_2(u)$ and $\eta(u, x_2) = 2(n - 3)$. $\square$

Now we prove Theorem 4. By Lemma 11, $\eta(K_n^2) = \eta(K_n^{n-2}) = 2n - 6$, and so Theorem 2 is a consequence of Theorem 4.

Proof of Theorem 4. Let G be a minimal counter-example to Theorem 4. Then G is a 2-connected non-complete graph on n vertices, $n \geq 4$, that is not isomorphic to K_n^2 or K_n^{n-2}, and Theorem 4 holds for any smaller graph satisfying the assumptions of the theorem. We note that $\eta(C_5) = 5$, thus G is not isomorphic to C_5.

By combining Lemmas 7 and 8, we infer that for any two vertices u, v in G such that $N[u] \subseteq N[v]$, the graph $G - u$ is not 2-connected or is complete. From Lemma 10, we have that there is a pair of vertices u, v in G such that $N[u] \subseteq N[v]$. Lemma 9 guarantees that $G - u$ is not 2-connected (v being the only cut-vertex in $G - u$) and no block of $G - u$ is complete or isomorphic to K_t^2 or K_t^{t-2} for any $t \in \mathbb{N}$. Let $C_1, \ldots, C_k$ be the blocks of $G - u$. Note that $k \geq 2$ and recall that v belongs to each of the blocks as $N[u] \subseteq N[v]$ and G is 2-connected. Let $G_i = G[V(C_i) \cup \{u\}]$ for every i, $1 \leq i \leq k$. Note that each G_i is a proper subgraph of G, it is 2-connected, and neither complete nor isomorphic to K_t^2 or K_t^{t-2} for any t (otherwise C_i is complete, or isomorphic to K_{t-1}^{t-3} or K_{t-1}^2, a contradiction). By minimality of G, we have $\eta(G_i) \geq 2|V(C_i)| - 5$ for every i.

We claim that

$$\eta(G) \geq \sum_{i=1}^{k} \eta(G_i) + \sum_{\{a,b\}} \big(g(a, b) - d(a, b) \big),$$

where the second sum runs over vertices a, b from distinct blocks of $G - u$. This follows from the fact that distances for vertices in G_i are left unchanged in G. Note that since u and v are counted in each G_i, it holds that

$$\sum_{i=1}^{k} \eta(G_i) \geq \sum_{i=1}^{k} \big(2|V(G_i)| - 5 \big) = 2n + 2 \cdot 2 \cdot (k - 1) - 5k = 2n - k - 4.$$

Since G is 2-connected, the vertex u has a neighbor w_i (distinct from v) in each block C_i. Since $N[u] \subseteq N[v]$, we have $g(w_i, w_j) - d(w_i, w_j) = 2$ for every $i \neq j$. Therefore

$$\sum_{\{a,b\}} \big(g(a, b) - d(a, b) \big) \geq 2 \binom{k}{2},$$

where again the sum runs over vertices a, b from distinct blocks. In total, to obtain $\eta(G) \geq 2n - 5$, all we need is $2\binom{k}{2} - k - 4 \geq -5$, i.e., $\binom{k}{2} \geq \frac{k-1}{2}$. This is always true as $k \geq 2$. $\square$

5. Additional results

In this section, we continue our analysis in order to prove several additional results regarding the difference between the Szeged and the Wiener index. Recall that $c_G(a)$ is a contribution of a to $\eta(G)$, see (2) and (3).

Lemma 12. *Let G be a connected graph with the blocks $B_1, \ldots, B_k$. Let $p_1, \ldots, p_k$ be integers such that for every i, with $1 \leq i \leq k$, it holds that $c_{G[B_i]}(u) \geq p_i$ for every vertex $u \in V(B_i)$. Then $c_G(u) \geq \Sigma_{1 \leq i \leq k} p_i$ for every vertex $u \in V$. In particular,*

$$\eta(G) \geq \frac{n}{2} \sum_{i=1}^{k} p_i.$$

Proof. Let u be a vertex of G. Without loss of generality, assume that $u \in V(B_1)$. Then $\sum_{v \in V(B_1) \setminus \{u\}} \eta(u, v) = \sum_{v \in V(B_1) \setminus \{u\}} \big(g(u, v) - d(u, v) \big) \geq p_1$. Now choose a block B_i, $2 \leq i \leq k$. Let $v \in V(B_i)$ and let w be a vertex of B_i which is at the shortest distance from u. Then w is a cut-vertex of G. Therefore, every edge xy being good for $\{w, v\}$ is also good for $\{u, v\}$, which implies $\sum_{v \in V(B_i) \setminus \{w\}} \eta(u, v) \geq \sum_{v \in V(B_i) \setminus \{w\}} \eta(w, v) \geq p_i$. Consequently, we infer $c_G(u) \geq \Sigma_{1 \leq i \leq k} p_i$. $\square$
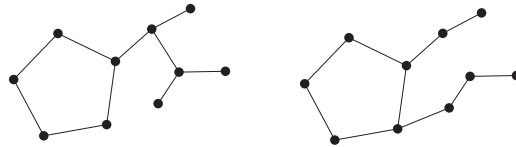
Fig. 2. Example of two graphs for which the difference between their Szeged and Wiener index attains $2n - 5$.

Lemmas 10 and 12 together imply the following theorem.

Theorem 13. *Let G be a connected graph with at least two blocks, neither of which is isomorphic to C_5 or a complete graph. Moreover, let G do not contain two vertices u, v with $N[u] \subseteq N[v]$. Then*

$$\eta(G) \geq 4n.$$

The following two theorems have been conjectured by the AutoGraphiX computer program [7], and confirmed in [2] and [3], respectively.

Theorem 14. [2] *Let G be a connected graph with $n \geq 5$ vertices, at least one odd cycle, and girth at least 5. Then*

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

Moreover, the equality holds if and only if the graph is composed of C_5 and a tree rooted at a vertex of C_5 or two trees rooted at two adjacent vertices of C_5 (Fig. 2).

Theorem 15. [3,2] *Let G be a connected bipartite graph with $n \geq 4$ vertices and $m \geq n$ edges. Then*

$$\eta(G) \geq 4n - 8.$$

Moreover, the equality holds if and only if the graph is composed of C_4 and a tree rooted at a vertex of C_4.

Additionally, Klavžar and Nadjafi-Arani [10] extended Theorems 14 and 15 in terms of the girth and the longest isometric cycle, respectively.

Using our approach, we are able to prove stronger versions of Theorems 14 and 15. First, we strengthen Theorem 14. Notice that the next statement requires girth 4 instead of 5.

Theorem 16. *Let G be a connected graph which has a triangle-free 2-connected block distinct from C_5, or at least two blocks isomorphic to C_5. Then*

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

Proof. Let B be a 2-connected block other than C_5 with girth at least 4. Then B is non-complete and it does not contain two vertices u, v with $N[u] \subseteq N[v]$. By Lemma 10, we have $c_B(u) \geq 4$ for every vertex $u \in V(B)$. On the other hand, $c_{C_5}(u) \geq 2$ for every vertex u of C_5. Consequently by Lemma 12, $c_G(u) \geq 4$ for every vertex u in a graph G satisfying the assumptions of theorem, which means that $\eta(G) \geq 2n$. $\square$

As a corollary, we obtain an alternative proof Theorem 14.

Alternative proof of Theorem 14. By Theorem 16, we have

$$\eta(G) \geq 2n > 2n - 5,$$

for every connected graph G with girth at least 4 and at least one 2-connected block distinct from C_5, or at least two blocks isomorphic to C_5. So, we may assume that G is a connected (unicyclic) graph with precisely one 2-connected block isomorphic to C_5.

Let $C = abcde$ be the C_5 in G, and let T_x, $x \in \{a, b, c, d, e\}$, be the component of $G \backslash E(C)$ containing x. Denote also $t_x = |V(T_x)|$. Obviously, $g(u, v) - d(u, v) = 0$ for every pair $u, v \in V(T_x)$. Observe also that for any pair of adjacent vertices $x, y \in V(C)$, it holds $g(u, v) - d(u, v) = 0$ for every $u \in V(T_x)$ and $v \in V(T_y)$. On the other hand, if $d(x, y) = 2$, then $g(u, v) - d(u, v) = 1$ for every $u \in V(T_x)$ and $v \in V(T_y)$. Since $t_a + t_b + t_c + t_d + t_e = n$, we have

$$\eta(G) = \mathrm{Sz}\,(G) - W(G) = t_a t_c + t_b t_d + t_c t_e + t_d t_a + t_e t_b$$
$$= n^2 - \frac{(t_a + t_b)^2}{2} - \frac{(t_b + t_c)^2}{2} - \frac{(t_c + t_d)^2}{2} - \frac{(t_d + t_e)^2}{2} - \frac{(t_e + t_a)^2}{2}. \tag{5}$$

We leave to the reader to verify that the minimum value of (5) is achieved in the case when at most two trees T_x and T_y, $x, y \in \{a, b, c, d, e\}$, have more than one vertex and x is adjacent to y. This completes the proof. $\square$

Now we consider bipartite graphs.

Theorem 17. *If G is a 2-connected bipartite graph, then either G is isomorphic to C_4 or $c(u) \geq 8$ for every vertex $u \in V$. In particular, if G is not isomorphic to C_4, then*

$$\eta(G) \geq 4n.$$

Proof. To prove the theorem, we will use analogous approach as in the proof of Lemma 10. Suppose, to the contrary, that a is a vertex of G with $c(a) \leq 7$. Consider a breadth-first-search tree of G rooted at a, with the levels $N_0, \ldots, N_p$.

Observe first that since G is bipartite, there are no two vertices u, v with $N[u] \subseteq N[v]$, no two vertices in a common level N_i are adjacent, and $p \geq 2$. Let $x \in N_p$. Then x has no neighbor in N_p. Let $y_1, \ldots, y_\ell$ be the neighbors of x in the previous level. Since G is 2-connected, $\ell \geq 2$. Let z_i be a neighbor of y_i in the level $f(x) - 2$. Note that z_i might be equal to z_j for some $i \neq j$. Anyway, the edges $z_i y_i$ and $y_i x$ are good for $\{a, x\}$, which gives $g(a, x) - d(a, x) \geq 2(\ell - 1) \geq 2$. Additionally, every edge $x y_j$ is good for $\{a, y_i\}$, if $i \neq j$, since $y_i y_j \notin E$. Thus, $g(a, y_i) - d(a, y_i) \geq \ell - 1 \geq 1$ for every i. The contribution of a is thus at least 4, and at least 10 if $\ell \geq 3$. It follows that x is the only vertex with two neighbors in the previous level, and moreover, it has precisely two such neighbors. Consequently $N_p = \{x\}$.

Consider now the levels $N_0, \ldots, N_{p-1}$. Since $G[N_i]$ is a graph without edges and x is the only vertex with at least two neighbors in the previous level, G is isomorphic to a cycle. It easy to calculate that in the case when $p \geq 3$, the contribution of a is at least 9. □

From Theorem 17 we also infer:

Theorem 18. *Let G be a connected graph which has a bipartite 2-connected block distinct from C_4, or at least two blocks isomorphic to C_4. Then*

$$\eta(G) \geq 4n.$$

Proof. If B is a block inducing a bipartite subgraph other than C_4, then $c_B(u) \geq 8$ for every vertex $u \in V(B)$, by Theorem 17. On the other hand, $c_{C_4}(u) \geq 4$ for every vertex u of C_4. Consequently by Lemma 12, $c_G(u) \geq 8$ for every vertex u in a graph G satisfying the assumptions of corollary, which means that $\eta(G) \geq 4n$. □

Similarly as above, we can derive Theorem 15 from Theorem 18.

Alternative proof of Theorem 15. By Theorem 18, we have

$$\eta(G) \geq 4n > 4n - 8,$$

for every bipartite connected graph G with at least one 2-connected block distinct from C_4, or at least two blocks isomorphic to C_4. So, we may assume that G is a bipartite connected (unicyclic) graph with precisely one 2-connected block isomorphic to C_4.

Let $C = abcd$ be the C_4 in G, and let T_x, $x \in \{a, b, c, d\}$, be the component of $G \setminus E(C)$ containing x. Denote also $t_x = |V(T_x)|$. Again, $g(u, v) - d(u, v) = 0$ for every pair $u, v \in V(T_x)$. For any pair of adjacent vertices $x, y \in V(C)$, it holds $g(u, v) - d(u, v) = 1$ for every $u \in V(T_x)$ and $v \in V(T_y)$. If $d(x, y) = 2$, then $g(u, v) - d(u, v) = 2$ for every $u \in V(T_x)$ and $v \in V(T_y)$. Thus,

$$\eta(G) = \mathrm{Sz}(G) - W(G) = t_a t_b + t_b t_c + t_c t_d + t_d t_a + 2(t_a t_c + t_b t_d)$$

$$= \frac{n^2 - (t_a - t_c)^2 - (t_b - t_d)^2}{2}. \tag{6}$$

It is straightforward to verify that the minimum value of (6) is achieved in the case when at most one tree T_x, $x \in \{a, b, c, d\}$, has more than one vertex. This completes the proof. □

6. Revised Szeged index

In this section, we consider a variation of the Szeged index. The *revised Szeged index* is defined as

$$\mathrm{Sz}^*(G) = \sum_{uv \in E} \left(n_{uv}(u) + \frac{n_0(u, v)}{2} \right) \left(n_{uv}(v) + \frac{n_0(u, v)}{2} \right),$$

where $n_0(u, v) = n - n_{uv}(u) - n_{uv}(v)$. Similarly as above, we define

$$\eta^*(G) = \mathrm{Sz}^*(G) - W(G).$$

For every vertex $a \in V$, we set $h(a)$ to be the number of edges horizontal to a. Note that

$$\sum_{a \in V} h(a) = \sum_{uv \in E} n_0(u, v).$$

Clearly, in every bipartite graph we have $\eta^*(G) = \eta(G)$. We therefore focus on non-bipartite graphs exclusively. Note that in a non-bipartite graph, it holds that $h(a) \geq 1$ for every vertex a.

A conjecture about the difference between the revised Szeged index and the Wiener index of a graph has also been proposed by AutoGraphiX [7] and confirmed by Chen et al. [2].

Theorem 19. [2] *Let G be a non-bipartite connected graph. Then*

$$\eta^*(G) \geq \frac{n^2}{4} + n - \frac{3}{2}.$$

Moreover, the equality is attained when the graph is composed of C_3 and a tree rooted at a vertex of C_3.

Recently, Klavžar and Nadjafi-Arani [11] extended the result in a way that it takes the number of edges into account. Here we present a similar result.

Lemma 20. *Let G be a non-bipartite connected graph. Then*

$$\eta^*(G) \geq \eta(G) + \frac{n^2}{4} + \frac{n}{2}.$$

More precisely, we have

$$\eta^*(G) \geq \eta(G) + \frac{n^2}{4} + \frac{n}{2} + \frac{n+2}{4} \cdot \sum_{a \in V} \left(h(a) - 1 \right).$$

Proof. We have

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

$$= \sum_{uv \in E} \left(n_{uv}(u) + \frac{n_0(u,v)}{2} \right) \left(n_{uv}(v) + \frac{n_0(u,v)}{2} \right) - \sum_{\{u,v\} \subseteq V} d(u,v)$$

$$= \sum_{uv \in E} \left(n_{uv}(u) n_{uv}(v) + \frac{n_0(u,v)}{2} \left(n_{uv}(v) + n_{uv}(u) + n_0(u,v) \right) - \frac{n_0(u,v)^2}{4} \right) - \sum_{\{u,v\} \subseteq V} d(u,v)$$

$$= \sum_{uv \in E} \left(n_{uv}(u) n_{uv}(v) \right) - \sum_{\{u,v\} \subseteq V} d(u,v) + \sum_{uv \in E} \left(\frac{n_0(u,v) \cdot n}{2} - \frac{n_0(u,v)^2}{4} \right)$$

$$= \eta(G) + \frac{1}{2} \sum_{uv \in E} n_0(u,v) \left(n - \frac{n_0(u,v)}{2} \right).$$

Note that $n_0(u,v) \leq n - 2$ for any edge uv, and so

$$\eta^*(G) \geq \eta(G) + \frac{1}{2} \sum_{uv \in E} n_0(u,v) \left(n - \frac{n-2}{2} \right)$$

$$= \eta(G) + \frac{n+2}{4} \sum_{uv \in E} n_0(u,v)$$

$$= \eta(G) + \frac{n+2}{4} \sum_{a \in V} h(a).$$

Recall that $h(a) \geq 1$ for any vertex a. Thus,

$$\eta^*(G) \geq \eta(G) + \frac{(n+2) \cdot n}{4} + \frac{n+2}{4} \sum_{a \in V} \left(h(a) - 1 \right).$$

$\square$

We use Lemma 20 to prove the following stronger version of Theorem 19.

Theorem 21. *Let G be a non-bipartite connected graph. Then*

$$\eta^*(G) \geq \frac{n^2}{4} + n,$$

unless G is obtained from a tree by expanding a single vertex into C_3.

Proof. Suppose, to the contrary, that G is a non-bipartite graph with $\eta^*(G) < \frac{n^2}{4} + n$. By Lemma 20, there is neither a vertex a with $h(a) \geq 3$, nor two vertices a, b with $h(a)$, $h(b) \geq 2$. In particular, G does not contain a diamond (a K_4 without one edge) as a subgraph, and hence G has no clique larger than a triangle. Similarly, the graph does not contain two edge-disjoint odd cycles. Therefore, there is at most one triangle in G.

Additionally, it holds that $\eta(G) < \frac{n}{2}$. By Lemma 12, no block satisfies $c(a) \geq 1$ for every vertex. Observe that every vertex u of C_5 satisfies $c(u) = 1$. Thus by Lemma 10, G does not contain 2-connected block without a triangle.

Hence, G has a unique 2-connected block B and this block contains a triangle. Suppose that there is a vertex a in B satisfying $c_B(a) = 0$. Moreover, suppose that a is not a dominating vertex in B. Then the breadth-first-search tree for B rooted

in a contains at least three levels. Since B is 2-connected, there must be in the last level either a vertex with two neighbors in the previous level or an edge whose endpoints are adjacent to two distinct neighbors in the previous level. Both these cases contradict to $c(a) = 0$. Hence, a is dominating in B. Since there is at most one triangle in B and B is 2-connected, we conclude that B is isomorphic to C_3. $\square$

Finding $\eta^*(G)$ for all graphs G obtained from a tree by expanding a single vertex into C_3 we obtain an alternative proof of Theorem 19.

Alternative proof of Theorem 19. By Theorem 21, we have

$$\eta^*(G) \geq \frac{n^2}{4} + n > \frac{n^2}{4} + n - \frac{3}{2}$$

for every connected non-bipartite graph G, unless G is obtained from a tree by expanding a single vertex into C_3. So, we may assume that G is a graph obtained from a tree by expanding one vertex into C_3.

Let $C = abc$ be the C_3 in G and let T_x, $x \in \{a, b, c\}$, be the component of $G \backslash E(C)$ containing x. Denote also $t_x = |V(T_x)|$. Then

$$\eta^*(G) = \mathrm{Sz}^*(G) - W(G) = \mathrm{Sz}^*(G) - \mathrm{Sz}(G) + \mathrm{Sz}(G) - W(G) = \mathrm{Sz}^*(G) - \mathrm{Sz}(G).$$

The last equality holds as G is a block graph. Note also that $n_0(u, v) = 0$, unless $uv \in \{ab, bc, ac\}$, in which cases it holds $n_0(a, b) = t_c$, $n_0(b, c) = t_a$, and $n_0(a, c) = t_b$. Since $n_x(x, y) = t_x$ for $x, y \in \{a, b, c\}$, $x \neq y$, we have

$$
\begin{aligned}
\eta^*(G) &= \sum_{uv \in E} \left(\left(n_u(uv) + \frac{n_0(u, v)}{2} \right) \left(n_v(uv) + \frac{n_0(u, v)}{2} \right) - n_u(uv) n_v(uv) \right) \\
&= \left(\left(n_a(ab) + \tfrac{1}{2} t_c \right) \left(n_b(ab) + \tfrac{1}{2} t_c \right) - n_a(ab) n_b(ab) \right) \\
&\quad + \left(\left(n_b(bc) + \tfrac{1}{2} t_a \right) \left(n_c(bc) + \tfrac{1}{2} t_a \right) - n_b(bc) n_c(bc) \right) \\
&\quad + \left(\left(n_a(ac) + \tfrac{1}{2} t_b \right) \left(n_c(ac) + \tfrac{1}{2} t_b \right) - n_a(ac) n_c(ac) \right) \\
&= \tfrac{1}{4} (t_a^2 + t_b^2 + t_c^2) + t_a t_b + t_a t_c + t_b t_c \\
&= \tfrac{5}{12} n^2 - \tfrac{1}{12} \left((t_a - t_b)^2 + (t_b - t_c)^2 + (t_c - t_a)^2 \right).
\end{aligned}
\tag{7}
$$

The minimum value of (7) is achieved when at most one tree T_x, $x \in \{a, b, c\}$, has more than one vertex. This completes the proof. $\square$

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