

On the Difference Between Wiener index and Graovac–Pisanski Index

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Abstract

Let G be a connected graph. The Wiener index of G is the sum of all distances in G , that is, $W(G) = \sum_{u,v \in V(G)} \text{dist}(u,v)$. On the other hand, the Graovac–Pisanski index of G is $\text{GP}(G) = \frac{|V(G)|}{2|\text{Aut}(G)|} \sum_{u \in V(G)} \sum_{\alpha \in \text{Aut}(G)} \text{dist}(u, \alpha(u))$, where $\text{Aut}(G)$ is the group of automorphisms of G . In this paper we study the difference $\Delta_W(G) = W(G) - \text{GP}(G)$. We show that this difference is nonnegative for trees, but there are graphs G for which $\Delta_W(G)$ is negative. We also find infinitely many graphs G which are not vertex-transitive and yet $\Delta_W(G) = 0$. For trees we completely determine the set of values of $\Delta_W(G)$.

1 Introduction

All graphs considered in this paper are connected. Let G be a graph. We denote the vertex and edge sets of G by $V(G)$ and $E(G)$, respectively. For two vertices u and v , by $\text{dist}(u,v)$ we denote the distance between u and v . Wiener index of a graph, $W(G)$, was

introduced by Wiener in [24]. It is the sum of distances between all (unordered) pairs of vertices in a graph, i.e.,

$$W(G) = \sum_{u,v \in V(G)} \text{dist}(u, v).$$

A great deal of knowledge on this index is accumulated in several survey papers [7, 8, 13, 14, 25].

Let G be a graph and let $U \subseteq V(G)$. The *Wiener index of U in G* is defined as the sum of distances between all vertex pairs in U

$$W_G(U) = \sum_{u,v \in U} \text{dist}(u, v).$$

Obviously, $W_G(V(G)) = W(G)$. Let $v \in V(G)$. By $w_U(v)$ we denote the sum of distances from v to all vertices of U . Hence,

$$w_U(v) = \sum_{u \in U} \text{dist}(u, v).$$

If $U = V(G)$, we write $w_G(v)$ instead of $w_{V(G)}(v)$. Using this notation one can rewrite the Wiener index as follows

$$W(G) = \frac{1}{2} \sum_{v \in V(G)} w_G(v).$$

Graovac-Pisanski index, $GP(G)$, of a graph was introduced in [10]. It is defined as

$$GP(G) = \frac{|V(G)|}{2|\text{Aut}(G)|} \sum_{u \in V(G)} \sum_{\alpha \in \text{Aut}(G)} \text{dist}(u, \alpha(u)),$$

where $\text{Aut}(G)$ is the group of automorphisms of G .

Graovac-Pisanski index (originally known as the modified Wiener index) presents an algebraic approach for generalizing the Wiener index. The definition of Graovac-Pisanski index is based on distances but its advantage is in considering also the symmetries of a graph. It is known that symmetries of a molecule have an influence on its properties [20]. Črepnjak et al. showed that the Graovac-Pisanski index of some hydrocarbon molecules is correlated with their melting points [5]. Graovac-Pisanski index was considered for nanostructures, linear polymers, and some classes of fullerenes and fullerene-like molecules [1–3, 17–19, 21–23].

Upper and lower bounds for Graovac-Pisanski index were considered in [18]. Graovac-Pisanski index was further considered from computational point of view in [9, 22]. Exact formulae for the Graovac-Pisanski index for some graph operations are present in [4]. Recent studies were devoted to identifying graphs with maximal values of this index among n -vertex trees and unicyclic graphs [15, 16].

The group of automorphisms of G partitions $V(G)$ into orbits. We say that $u, v \in V(G)$ belong to the same *orbit* if there is an automorphism $\alpha \in \text{Aut}(G)$ such that $\alpha(u) = v$. Let V_1, V_2, \dots, V_t be all the orbits of $\text{Aut}(G)$ in G . In [10] it was shown that for every graph G

$$\text{GP}(G) = |V(G)| \cdot \sum_{i=1}^t \frac{W_G(V_i)}{|V_i|}, \quad (1)$$

where V_1, V_2, \dots, V_t are the orbits of $\text{Aut}(G)$. Since all vertices u in an orbit U have the same value of $w_U(u)$, we can rewrite (1) in the following way (see [6])

$$\text{GP}(G) = \frac{|V(G)|}{2} \cdot \sum_{i=1}^t w_{V_i}(v_i), \quad (2)$$

where V_1, V_2, \dots, V_t are the orbits of $\text{Aut}(G)$ and v_1, v_2, \dots, v_t , respectively, are their representatives. Using (2) one can see that the Graovac-Pisanski index of every graph is either an integer or half of an integer number. Moreover, in [6] it was shown that for bipartite graphs the following statement holds.

Proposition 1. *If G is a bipartite graph then $\text{GP}(G)$ is an integer number.*

Since trees are bipartite graphs, Proposition 1 implies that $\text{GP}(T)$ is an integer number if T is a tree. If a graph has no nontrivial automorphisms, that is if all its orbits consist of single vertices, then its Graovac-Pisanski index is 0.

Some researchers have shown interest in the difference between Wiener index and Graovac-Pisanski index. Denote

$$\Delta_W(G) = W(G) - \text{GP}(G).$$

This difference was first considered in [11], and in [12] it was computed for some families of polyhedral graphs. In both these papers one can find an erroneous statement that a graph G is vertex-transitive if and only $\Delta_W(G) = 0$. It was observed already in [10] that for a vertex-transitive graph $\Delta_W(G) = 0$, however we find infinitely many graphs G which are not vertex-transitive and yet $\Delta_W(G) = 0$, see Section 2. In the same section we show that there exist graphs G for which $\Delta_W(G)$ is negative. In the last section we prove that $\Delta_W(G)$ is nonnegative for trees. Moreover, we completely determine the set of values of $\Delta_W(G)$ if G is a tree.

2 General graphs

Let G be a graph. As already mentioned, $\text{GP}(G) = W(G)$ if G is vertex-transitive, i.e., if there is just one orbit of vertices of $\text{Aut}(G)$. On the other hand, if G has $|V(G)|$

orbits of $\text{Aut}(G)$ then $\text{GP}(G) = 0$. Regarding the number of orbits these two cases are extremal, and so maybe one could expect that $0 \leq \text{GP}(G) \leq W(G)$. While the inequality $0 \leq \text{GP}(G)$ follows from the definition and it is obvious that $\text{GP}(G) = 0$ if and only if G has $|V(G)|$ orbits, the inequality $\text{GP}(G) \leq W(G)$ is not so obvious although one can object that all the distases contribute to $W(G)$ while only some of them contribute to $\text{GP}(G)$. The problem is caused by the normalizing factors $|V(G)|$ and $\frac{1}{|V_i|}$ in (1). From the terms in (1) one can deduce that $\Delta_W(G) = W(G) - \text{GP}(G)$ can be negative if there are “big distances” inside orbits and “small distances” between them. A typical example of such a situation is a complete bipartite graph $K_{a,b}$, where $a \neq b$. We have the following statement.

Proposition 2. *Let $a > b \geq 1$. Then*

$$\Delta_W(K_{a,b}) = a + b - ab.$$

Proof. Let $a > b \geq 1$. In $K_{a,b}$, denote by V_1 and V_2 the partite sets with a and b vertices, respectively. Further, let $v_1 \in V_1$ and $v_2 \in V_2$. Then

$$\begin{aligned} w_G(v_1) &= 2(a-1) + b, & w_{V_1}(v_1) &= 2(a-1), \\ w_G(v_2) &= 2(b-1) + a & w_{V_2}(v_2) &= 2(b-1). \end{aligned}$$

Hence we have

$$\begin{aligned} W(K_{a,b}) &= \frac{1}{2} \cdot a(2a + b - 2) + \frac{1}{2} \cdot b(a + 2b - 2) = a^2 + b^2 + ab - a - b, \\ \text{GP}(G) &= (a + b)\left(\frac{1}{2} \cdot 2(a-1) + \frac{1}{2} \cdot 2(b-1)\right) = a^2 + b^2 + 2ab - 2a - 2b, \end{aligned}$$

and so $\Delta_W(K_{a,b}) = a + b - ab$. ■

Observe that $\Delta_W(K_{a,1}) = 1$. However, if $b \geq 2$ then

$$a + b - ab = b - (b-1)a \leq b - a < 0.$$

Hence, we obtain the following corollary.

Corollary 3. *For every $n \geq 5$ there is a graph G on n vertices such that*

$$\Delta_W(G) < 0.$$

It is easy to check that all connected graphs G on $n \leq 4$ vertices satisfy $\Delta_W(G) \geq 0$. But Corollary 3 naturally opens the following problem.

Problem 4. *Let G be a graph on n vertices. What is the minimum value of $\Delta_W(G)$?*

Denote by $m(n)$ the minimum value of $\Delta_W(G)$ from Problem 4. For $K_{a,b}$ we cannot have $a = b$. Therefore, the minimum value of $\Delta_W(K_{a,b})$ occurs when $a - (n-a) = 1$ or $a - (n-a) = 2$ depending on the parity of n . Hence,

$$\begin{aligned} m(n) &\leq n + \frac{1}{4} - \frac{n^2}{4} && \text{if } n \text{ is odd,} \\ m(n) &\leq n + 1 - \frac{n^2}{4} && \text{if } n \text{ is even.} \end{aligned}$$

However, it is not known whether these bounds are tight.

Now we turn our attention to graphs G for which $\Delta_W(G) = 0$. Observe that $a+b-ab = 0$ is equivalent to $a = \frac{b}{b-1}$ for $b \geq 2$. Since a is an integer we get $b = 2$, implying $a = b$, which is false. Hence, there are no $a > b \geq 1$ such that $\Delta_W(K_{a,b}) = 0$. But there are graphs G which are not vertex-transitive and yet $\Delta_W(G) = 0$.

Let A, B and C be disjoint sets having a, b and c vertices, respectively. We define a graph $G_{a,b,c}$ as follows. $V(G_{a,b,c}) = A \cup B \cup C$ and $e = uv$ is an edge of $G_{a,b,c}$ if and only if either $u \in A$ and $v \in B$, or $u \in B$ and $v \in C$, or $u, v \in C, u \neq v$. In fact, $G_{a,b,c}$ is $(D_a \oplus K_c) + D_b$ where D_n is an empty graph on n vertices, K_n is a complete graph on n vertices, \oplus denotes the disjoint union and $+$ denotes the join of graphs. Since $G_{a,b,1}$ is $K_{a+1,b}$, we require $c \geq 2$. We have the following statement.

Lemma 5. *Let $a, b \geq 1$ and $c \geq 2$. Then*

$$\Delta_W(G_{a,b,c}) = \frac{1}{2}(-2ab + ac - bc + 3a + 3b + 4c).$$

Proof. Observe that A, B and C are the orbits of $\text{Aut}(G_{a,b,c})$. Let $u \in A, v \in B$ and $z \in C$. We have

$$\begin{aligned} w_G(\bar{u}) &= 2(a-1) + b + 2c, & w_A(u) &= 2(a-1), \\ w_G(v) &= a + 2(b-1) + c, & w_B(v) &= 2(b-1), \\ w_G(z) &= 2a + b + (c-1), & w_C(z) &= (c-1). \end{aligned}$$

Hence

$$\begin{aligned} W(G_{a,b,c}) &= \frac{1}{2}(a(2a+b+2c-2) + b(a+2b+c-2) + c(2a+b+c-1)) \\ &= \frac{1}{2}(2a^2 + 2b^2 + c^2 + 2ab + 4ac + 2bc - 2a - 2b - c) \\ \text{GP}(G_{a,b,c}) &= \frac{1}{2}(a+b+c)((2a-2) + (2b-2) + (c-1)) \\ &= \frac{1}{2}(2a^2 + 2b^2 + c^2 + 4ab + 3ac + 3bc - 5a - 5b - 5c) \end{aligned}$$

which gives $\Delta_W(G_{a,b,c})$ as required. ■

Observe that if $a = b$ then

$$\Delta_W(G_{a,b,c}) = 3a - a^2 + 2c.$$

Hence if $c = \frac{a^2-3a}{2}$ we get $\Delta_W(G_{a,a,c}) = 0$. The expression $a^2 - 3a$ is even for every value of a but $c \geq 2$ implies $a \geq 4$. So we have the following corollary.

Corollary 6. *Let $a \geq 4$ and let $c = \frac{a^2-3a}{2}$. Then $\Delta_W(G_{a,a,c}) = 0$.*

Corollary 6 gives an infinite class of graphs G which are not vertex-transitive and yet $W(G) = \text{GP}(G)$. The problem, for which values n there are non-vertex-transitive graphs G on n vertices such that $\Delta_W(G) = 0$, remains open.

3 Trees

If $e \in E(G)$, then $G - e$ denotes the graph with vertex set $V(G)$ and edge set $E(G) \setminus \{e\}$. As shown in [24], if G is a tree, then its Wiener index can be computed using the following lemma.

Lemma 7. *Let T be a tree. For every edge e in T , denote by $n(e)$ and $n'(e)$ orders of the two trees of $T - e$. Then*

$$W(T) = \sum_{e \in E(T)} n(e) \cdot n'(e).$$

In Lemma 7, every summand counts how many times an edge occurs on a (shortest, and unique) path connecting two vertices of $V(T)$. Therefore, we have the following analogue of Lemma 7 for $W_G(U)$.

Lemma 8. *Let T be a tree and let $U \subseteq V(T)$. For every edge e in T , denote by $n_U(e)$ and $n'_U(e)$, respectively, the number of vertices of U in the two trees of $T - e$. Then*

$$W_T(U) = \sum_{e \in E(T)} n_U(e) \cdot n'_U(e).$$

By P_n we denote a path on n vertices. Since every tree has at most two central vertices and since vertices which are central cannot be in the same orbit as non-central ones, P_1 and P_2 are the only trees which have just one orbit of the group of automorphisms, i.e., which are vertex-transitive. Hence, $W(T) = \text{GP}(T)$ if T is P_1 or P_2 . For all other trees the following statement is true.

Theorem 9. *Let T be a tree on at least three vertices. Then*

$$W(T) > \text{GP}(T).$$

Proof. By (1) we have to prove

$$W(T) > |V(T)| \cdot \sum_{i=1}^t \frac{W_T(V_i)}{|V_i|}, \quad (3)$$

where V_1, V_2, \dots, V_t are the orbits of $\text{Aut}(T)$. We prove this statement using Lemma 8. Fix an endvertex of T and denote it by q . For every $U \subseteq V(T)$, by $n_U(e)$ we denote the number of vertices of U in the component of $T - e$ containing q , while $n'_U(e)$ is the number of vertices of U in the other component of $T - e$. For every orbit V_i of $\text{Aut}(T)$, let $n_i = |V_i|$ and let $a_i(e) = n_{V_i}(e)$. Then $n'_{V_i}(e) = n_i - a_i(e)$. Since $n_{V(G)}(e) = \sum_{i=1}^t a_i(e)$, $n'_{V(G)}(e) = \sum_{i=1}^t (n_i - a_i(e))$ and $|V(T)| = \sum_{i=1}^t n_i$, after reordering the sums, (3) is equivalent to

$$\sum_{e \in E(T)} \left(\sum_{i=1}^t a_i(e) \cdot \sum_{i=1}^t (n_i - a_i(e)) \right) > \sum_{e \in E(T)} \sum_{i=1}^t n_i \cdot \left(\sum_{i=1}^t \frac{a_i(e) \cdot (n_i - a_i(e))}{n_i} \right)$$

Hence, (3) is true if for every edge e we have

$$\sum_{i=1}^t a_i(e) \cdot \sum_{i=1}^t (n_i - a_i(e)) \geq \sum_{i=1}^t n_i \cdot \sum_{i=1}^t \frac{a_i(e) \cdot (n_i - a_i(e))}{n_i}$$

and for at least one edge the inequality is strict.

So let $e \in E(T)$. Denote $p_i = a_i(e)/n_i$, $1 \leq i \leq t$. Then $0 \leq p_i \leq 1$. Observe that $0 \leq (p_i - p_j)^2$ and equality holds if and only if $p_i = p_j$. Hence,

$$0 \leq \sum_{1 \leq i < j \leq t} n_i n_j (p_i - p_j)^2 \quad (4)$$

and equality holds if and only if $p_1 = p_2 = \dots = p_t$. However, (4) is equivalent to the following

$$\begin{aligned} \sum_{i=1}^t n_i^2 p_i^2 + \sum_{1 \leq i < j \leq t} 2n_i n_j p_i p_j &\leq \sum_{i=1}^t n_i^2 p_i^2 + \sum_{1 \leq i < j \leq t} (n_i n_j p_i^2 + n_i n_j p_j^2) \\ \sum_{i=1}^t n_i p_i \cdot \sum_{i=1}^t n_i p_i &\leq \sum_{i=1}^t n_i \cdot \sum_{i=1}^t n_i p_i^2 \\ \sum_{i=1}^t n_i p_i \cdot \sum_{i=1}^t n_i - \sum_{i=1}^t n_i p_i \cdot \sum_{i=1}^t n_i p_i &\geq \sum_{i=1}^t n_i \cdot \sum_{i=1}^t n_i p_i - \sum_{i=1}^t n_i \cdot \sum_{i=1}^t n_i p_i^2 \\ \sum_{i=1}^t n_i p_i \cdot \sum_{i=1}^t (n_i - n_i p_i) &\geq \sum_{i=1}^t n_i \cdot \sum_{i=1}^t n_i p_i (1 - p_i) \\ \sum_{i=1}^t a_i(e) \cdot \sum_{i=1}^t (n_i - a_i(e)) &\geq \sum_{i=1}^t n_i \cdot \sum_{i=1}^t \frac{a_i(e) \cdot (n_i - a_i(e))}{n_i} \end{aligned} \quad (5)$$

and equality holds in (5) if and only if $\frac{a_1(e)}{n_1} = \frac{a_2(e)}{n_2} = \dots = \frac{a_t(e)}{n_t}$.

Let $e^* = qu$, where q is the fixed endvertex. Since T has at least three vertices, q and u have different degrees, and so they belong to different orbits of $\text{Aut}(T)$. Assume that $q \in V_1$ and $u \in V_2$. Then $n_{V_1}(e^*) = a_1(e^*) = 1$ while $n_{V_2}(e^*) = a_2(e^*) = 0$. Hence $p_1 = a_1(e^*)/n_1 > 0$ while $p_2 = a_2(e^*)/n_2 = 0$. So in this case we have a strict inequality in (5) which proves (3). ■

Now we find the values of $\Delta_W(T)$, when T is a tree. For this we need to calculate Δ_W for four types of trees, namely T_a^1 , $T_{a,b}^1$, T_a^2 and $T_{a,b}^2$. The graphs T_a^1 and $T_{a,b}^1$ have one central vertex, say c . T_a^1 is obtained when a pendant vertices are attached to c , where $a \geq 2$. Hence, T_a^1 is the star $K_{a,1}$. $T_{a,b}^1$ is obtained from T_a^1 by attaching b pendant vertices to every endvertex of T_a^1 , where $b \geq 1$. Observe that $T_{a,b}^1$ has $1 + a + ab$ vertices. The graphs T_a^2 and $T_{a,b}^2$ have two adjacent central vertices, say c_1 and c_2 . T_a^2 is obtained from the edge c_1c_2 by attaching a pendant vertices to each endvertex of c_1c_2 , where $a \geq 1$. So T_a^2 has $2 + 2a$ vertices. $T_{a,b}^2$ is obtained from T_a^2 by attaching b pendant vertices to every endvertex of T_a^2 , where $b \geq 1$. Observe that $T_{a,b}^2$ has $2 + 2a + 2ab$ vertices. We have the following lemma.

Lemma 10. *We have*

$$\begin{aligned} \Delta_W(T_a^1) &= 1, & \Delta_W(T_{a,b}^1) &= 2 + a + b, \\ \Delta_W(T_a^2) &= 2, & \Delta_W(T_{a,b}^2) &= 4 + 2a + 2b. \end{aligned}$$

Proof. By Proposition 2, $\Delta_W(T_a^1) = 1$, so we consider only $T_{a,b}^1$, T_a^2 and $T_{a,b}^2$ here. Let T be a tree with orbits V_1, V_2, \dots, V_t , where $n_i = |V_i|$ for $1 \leq i \leq t$, and for $e \in E(T)$ let

$$\Delta_W(e) = \sum_{i=1}^t a_i(e) \cdot \sum_{i=1}^t (n_i - a_i(e)) - \sum_{i=1}^t n_i \cdot \sum_{i=1}^t \frac{a_i(e) \cdot (n_i - a_i(e))}{n_i},$$

where $a_1(e), a_2(e), \dots, a_t(e)$ are numbers of vertices of V_1, V_2, \dots, V_t , respectively, in the component of $T - e$ containing a specific vertex q . As shown in the proof of Theorem 9,

$$\Delta_W(T) = \sum_{e \in E(T)} \Delta_W(e).$$

Observe that this specific vertex q can be chosen for every edge e separately, important is only that all $a_1(e), a_2(e), \dots, a_t(e)$ relate to the same component of $T - e$.

The graph $T_{a,b}^1$ has exactly three orbits of vertices. Let V_1 be the orbit of endvertices of $T_{a,b}^1$, let V_2 be the orbit of vertices adjacent to endvertices and let $V_3 = \{c\}$. Further, let e_1 be a pendant edge and let e_2 be an edge incident with c . For computing $\Delta_W(e_1)$,

we choose q to be the endvertex of e_1 of degree 1, and to obtain $\Delta_W(e_2)$ let q be the endvertex of e_2 different from c . Then

$$\begin{aligned}\Delta_W(e_1) &= 1 \cdot (a+ab) - (1+a+ab) \left(\frac{1 \cdot (ab-1)}{ab} + \frac{0 \cdot a}{a} + \frac{0 \cdot 1}{1} \right) = \frac{1+a}{ab}, \\ \Delta_W(e_2) &= (1+b) \cdot (a-b+ab) - (1+a+ab) \left(\frac{b \cdot (ab-b)}{ab} + \frac{1 \cdot (a-1)}{a} + \frac{0 \cdot 1}{1} \right) = \frac{1+b}{a}.\end{aligned}$$

Since $T_{a,b}^1$ has ab edges like e_1 (that is, incident with a pendant vertex) and a edges like e_2 , we have $\Delta_W(T_{a,b}^1) = 2 + a + b$.

Analogously, the graph T_a^2 has exactly two orbits of vertices. Let V_1 be the orbit of endvertices of T_a^2 and let $V_2 = \{c_1, c_2\}$. Further, let e be a pendant edge. Then

$$\Delta_W(e) = 1 \cdot (1 + 2a) - (2 + 2a) \left(\frac{1 \cdot (2a-1)}{2a} + \frac{0 \cdot 2}{2} \right) = \frac{1}{a},$$

while $\Delta_W(c_1c_2) = 0$ since $a_i(c_1c_2)/n_i = \frac{1}{2}$ for $1 \leq i \leq 2$ in this case. Since T_a^2 has $2a$ pendant edges, we get $\Delta_W(T_a^2) = 2$.

The graph $T_{a,b}^2$ has three orbits of vertices. Let V_1 be the orbit of endvertices of $T_{a,b}^2$, let V_2 be the orbit of vertices adjacent to endvertices and let $V_3 = \{c_1, c_2\}$. Further, let e_1 be a pendant edge and let e_2 be an edge incident with a central vertex, $e \neq c_1c_2$. Then

$$\begin{aligned}\Delta_W(e_1) &= 1 \cdot (1+2a+2ab) - (2+2a+2ab) \left(\frac{1 \cdot (2ab-1)}{2ab} + \frac{0 \cdot 2a}{2a} + \frac{0 \cdot 2}{2} \right) = \frac{1+a}{ab}, \\ \Delta_W(e_2) &= (1+b) \cdot (1+2a-b+2ab) - (2+2a+2ab) \left(\frac{b \cdot (2ab-b)}{2ab} + \frac{1 \cdot (2a-1)}{2a} + \frac{0 \cdot 2}{2} \right) \\ &= \frac{1+b}{a},\end{aligned}$$

while $\Delta_W(c_1c_2) = 0$ since $a_i(c_1c_2)/n_i = \frac{1}{2}$ for $1 \leq i \leq 3$ in this case. Since $T_{a,b}^2$ has $2ab$ edges like e_1 and $2a$ edges like e_2 , we have $\Delta_W(T_{a,b}^2) = 2 + 2a + 2 + 2b = 4 + 2a + 2b$. ■

Using Lemma 10 we can prove the following theorem.

Theorem 11. *There exists a tree T satisfying $\Delta_W(T) = \ell$ if and only if ℓ is integer, $\ell \geq 0$ and $\ell \notin \{3, 4\}$.*

Proof. By Proposition 1 and Theorem 9, we have that ℓ is a nonnegative integer.

Since the paths P_1 and P_2 are vertex-transitive, $\Delta_W(P_1) = \Delta_W(P_2) = 0$. By Lemma 10, $\Delta_W(T_a^1) = 1$ and $\Delta_W(T_a^2) = 2$. Further, $\Delta_W(T_{a,b}^1) = 2 + a + b$, where $a \geq 2$ and $b \geq 1$. Hence, if $\ell \geq 5$ then $\Delta_W(T_{\ell-3,1}^1) = \ell$ since $\ell - 3 \geq 2$. In the rest of the proof we show that ℓ cannot be 3 or 4.

So let T be a tree such that $\Delta_W(T) = 3$ or $\Delta_W(T) = 4$. Further, let V_i be an orbit containing only pendant vertices of T . Observe that V_i does not need to contain all

pendant vertices of T . As in the previous proofs, denote $n_i = |V_i|$. Let e be an edge containing a vertex of V_i . Then its contribution to $\Delta_W(T)$ is

$$\Delta_W(e) = 1 \cdot (n - 1) - n \cdot \frac{1 \cdot (n_i - 1)}{n_i} = \frac{n - n_i}{n_i},$$

where $n = |V(T)|$. Since there are exactly n_i edges with one endvertex in V_i , these edges contribute to $\Delta_W(T)$ by $n - n_i$.

Now suppose that there are two distinct orbits, say V_1 and V_2 , containing (possibly not all) endvertices of T . Then pendant edges contribute to $\Delta_W(T)$ by at least $(n - n_1) + (n - n_2) = 2n - n_1 - n_2$. Since $\Delta_W(T) \neq 0$, T has at least three vertices, and so the central vertex of T cannot be pendant. Denote by k the number of vertices of T which are not in $V_1 \cup V_2$, i.e. $k = n - n_1 - n_2$. Then the pendant edges contribute to $\Delta_W(T)$ by at least $n + k$. Since $n \geq 3$ and $k \geq 1$, we have $n + k \geq 4$ and equality holds only if T has exactly three vertices. But then T is P_3 and all endvertices of T belong to one orbit of $\text{Aut}(T)$, a contradiction.

So all endvertices of T belong to a single orbit of $\text{Aut}(T)$, say V_1 . Observe that if there are at least five vertices in T which are not pendant, then $n_1 \leq n - 5$ and so the pendant edges contribute to $\Delta_W(T)$ by at least 5, a contradiction. Hence, deleting all endvertices of T results in a tree T' which has at most 4 vertices. To complete the proof we distinguish 5 cases according to the structure of T' .

Case 1: $|V(T')| = 1$. In this case T is T_a^1 for some $a \geq 2$, and so $\Delta_W(T) = 1$, by Lemma 10.

Case 2: $|V(T')| = 2$. Then T is T_a^2 for some $a \geq 1$, and so $\Delta_W(T) = 2$, by Lemma 10.

Case 3: $|V(T')| = 3$. Then T' is the path P_3 . The graph T is obtained from T' by attaching pendant vertices to both endvertices of P_3 and possibly also to the central vertex of P_3 . But since there is only one orbit of pendant vertices in T , there are no pendant vertices adjacent to the central vertex of P_3 . Hence, T is $T_{2,b}^1$ for some $b \geq 1$. Consequently, $\Delta_W(T) = 2 + 2 + b \geq 5$, by Lemma 10.

Case 4: $|V(T')| = 4$ and T' is the path P_4 . Then analogously as above one can show that T is $T_{1,b}^2$ for some $b \geq 1$. But then $\Delta_W(T) = 4 + 2 + 2b \geq 8$, by Lemma 10.

Case 5: $|V(T')| = 4$ and T' is the claw T_3^1 . Then T is $T_{3,b}^1$ for some $b \geq 1$, which means that $\Delta_W(T) = 2 + 3 + b \geq 6$, by Lemma 10.

Since we obtained a contradiction in all cases, the proof is complete. ■

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