Partition distance in graphs

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Abstract

If G is a graph and $\mathcal{P}$ is a partition of $V(G)$, then the partition distance of G is the sum of the distance between all pairs of vertices that lie in the same part of $\mathcal{P}$. This concept generalizes several metric concepts and is dual to the concept of the colored distance due to Dankelmann, Goddard, and Slater. It is proved that the partition distance of a graph can be obtained from the Wiener index of weighted quotient graphs induced by the transitive closure of the Djoković-Winkler relation as well as by any partition coarser than it. It is demonstrated that earlier results follow from the obtained theorems. Applying the main results, upper bounds on the partition distance of trees with prescribed order and radius are proved and corresponding extremal trees characterized.

Keywords: partition distance; Djoković-Winkler relation; weighted graph; Wiener index; tree

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1 Introduction

Let G be a graph and let $\mathcal{P} = \{V_1, \ldots, V_k\}$ be a partition of $V(G)$. Let $f_{\mathcal{P}} : V(G) \to [k] = \{1, \ldots, k\}$ be the index function of $\mathcal{P}$ defined with $f_{\mathcal{P}}(v) = i$, where $v \in V_i$. The *Wiener index* $W(G)$ of G, defined as the sum of the distances between all unordered pairs of vertices of G, can be decomposed with respect to $\mathcal{P}$ as

$$W(G) = \sum_{\substack{\{u,v\} \\ f_{\mathcal{P}}(u)=f_{\mathcal{P}}(v)}} d_G(u,v) + \sum_{\substack{\{u,v\} \\ f_{\mathcal{P}}(u)\neq f_{\mathcal{P}}(v)}} d_G(u,v)\,.$$

An equivalent approach to the Wiener index of a graph is to study its average distance, cf. [24].) Denoting the above sums with $W_{\mathcal{P}}(G)$ and $W_{\overline{\mathcal{P}}}(G)$, respectively, the Wiener index of G thus decomposes as

$$W(G) = W_{\mathcal{P}}(G) + W_{\overline{\mathcal{P}}}(G)\,. \tag{1}$$

We call $W_{\mathcal{P}}(G)$ the *partition distance* of G (with respect to $\mathcal{P}$). The function $W_{\overline{\mathcal{P}}}(G)$ was earlier introduced by Dankelmann, Goddard, and Slater [4] as the *colored distance* of G (with respect to $\mathcal{P}$) with a location problem from [14] as a motivation. In this problem one aims to partition the nodes of a network considered into a set of facility nodes and a set of customer nodes, such that the average distance between a facility and a customer is minimized. Clearly, if $|\mathcal{P}| = |V(G)|$, then $W_{\overline{\mathcal{P}}}(G) = W(G)$ and if $|\mathcal{P}| = 1$, then $W_{\overline{\mathcal{P}}}(G) = 0$. Moreover, the so-called (un-weighted) *median problem* (cf. [12]) asks to determine a partition $\mathcal{P} = \{V_1, V_2\}$, where $|V_1| = 1$, such that $W_{\overline{\mathcal{P}}}(G)$ is smallest possible.

Several invariants of wide interest in chemical graph theory can be expressed as instances of the partition distance. First of all, if $|\mathcal{P}| = 1$, then $W_{\mathcal{P}}(G) = W(G)$. Consider next a fixed positive integer k and a graph G with vertices $v_1, \ldots, v_n$, where $\deg(v_1) = \cdots = \deg(v_r) = k$ and $\deg(v_i) \neq k$ for any $i > r$. Then setting $\mathcal{P} = \{\{v_1, \ldots, v_r\}, \{v_{r+1}\}, \ldots, \{v_n\}\}$ we have

$$W_{\mathcal{P}}(G) = TW_k(G)\,,$$

where $TW_k(G)$ is the *generalized terminal Wiener index* of G due to Ilić and Ilić [16]. $TW_k(G)$ in turn extends the *terminal Wiener index* $TW(G) = TW_1(G)$ introduced in [11], see also [3, 22]. As another special case of the partition distance, if no condition is imposed on the first part of the partition $\mathcal{P}$, the partition distance coincides with the concept of the relative Wiener index from [2]. Moreover, some basic graph invariants can also be expressed using the partition distance. Let us give two examples here. If G is a graph with vertices $v_1, \ldots, v_n$, where $d(v_1, v_2) = \mathrm{diam}(G)$, then by setting $\mathcal{P} = \{\{v_1, v_2\}, \{v_3\}, \ldots, \{v_n\}\}$ we have $W_{\mathcal{P}}(G) = \mathrm{diam}(G)$. And if $v_1, \ldots, v_n$ are vertices of G such that $v_1, \ldots, v_{\omega(G)}$ induce a largest clique of G, then by setting $\mathcal{P} = \{\{v_1, \ldots, v_{\omega(G)}\}, \{v_{\omega(G)+1}\}, \ldots, \{v_n\}\}$, the clique number $\omega(G)$ of G can be written as $\omega(G) = \left(1 + \sqrt{1 + 8W_{\mathcal{P}}(G)}\right)/2$.

In the next section we prove our main results which assert that the partition distance of a graph can be obtained from certain smaller weighted graphs. We also show that numerous earlier results follow directly from the obtained theorems. Then, in Section 3, different general upper bounds on the partition distance of trees are proved. Trees that attain the respective bounds are also characterized. The obtained bounds are also applied to the (generalized) terminal Wiener index. We conclude with some remarks on the relation between the partition distance and the colored distance and on the concept of the k-diameter from [8].

2 Partition distance from Θ^*-quotient graphs

In this section we first prove that the partition distance of a graph can be obtained as the sum of the Wiener indexes of weighted quotient graphs induced by the Θ^*- relation; see Theorem 2.2. Then, in Theorem 2.3, we observe that the same conclusion holds for any partition that is coarser than the Θ^*-partition. We close the section by listing several known results that are consequences of these theorems.

Recall that the edges $e = xy$ and $f = uv$ of a connected graph G are in the *Djoković-Winkler relation* Θ [5, 25] if $d_G(x,u) + d_G(y,v) \neq d_G(x,v) + d_G(y,u)$. The transitive closure Θ^* of Θ is an equivalence relation on $E(G)$, the corresponding partition is called the Θ^*-*partition*. In the next result we collect those results from [9] (see also [17, Lemmas 14.1, 14.2, 14.3]) that we will make use of.

Lemma 2.1 *(i) Let P be a shortest path in G. Then no two edges of P are in the relation Θ.*

(ii) Let $e = uv$ be an edge of a graph G, and let W be a u,v-walk in G that does not contain e. Then there exists an edge f of W such that $e\Theta f$.

(iii) Let F be a Θ^*-class of a connected graph G, and let $u, v \in V(G)$. If P is a shortest u,v-path and Q an arbitrary u,v-path, then $|Q \cap F| \geq |P \cap F|$.

Let G be a connected graph and let $\{F_1, \ldots, F_r\}$ be a partition of $E(G)$. For any $i \in [r]$, the *quotient graph* G/F_i has the connected components of the graph $G - F_i$ as vertices, components C and C' being adjacent if there exists an edge $uv \in F_i$ such that $u \in C$ and $v \in C'$. A *weighted graph* (G, w) means a vertex-weighted graph, that is, a graph G together with the weight function $w : V(G) \to \mathbb{R}_0^+$. The Wiener index $W(G, w)$ of the weighted graph (G, w) was introduced in [18] as:

$$W(G,w) = \sum_{\{x,y\} \in \binom{V(G)}{2}} w(x)w(y)d_G(x,y)\,.$$

If $w \equiv 1$, then $W(G, w) = W(G)$. Now all is ready for our main result.

Theorem 2.2 *Let G be a connected graph and let $\mathcal{P} = \{V_1, \ldots, V_k\}$ be a partition of $V(G)$. If $\{F_1, \ldots, F_r\}$ is the Θ^*-partition of $E(G)$, then*

$$W_{\mathcal{P}}(G) = \sum_{i=1}^{r}\sum_{j=1}^{k} W(G/F_i, w_i^{(j)})\,,$$

where $w_i^{(j)}(C) = |C \cap V_j|$ for any $C \in V(G/F_i)$.

Proof. For any vertices $x, y \in V(G)$, $x \neq y$, that belong to some V_j, $j \in [k]$, select a shortest x,y-path and denote it with $P_{x,y}$. Counting the edges of all the selected paths we have:

$$W_{\mathcal{P}}(G) = \sum_{j=1}^{k} \sum_{\{x,y\}\in\binom{V_j}{2}} |E(P_{x,y})| \,. \tag{2}$$

Consider an arbitrary pair $\{x, y\} \in \binom{V_j}{2}$ and assume that $|P_{x,y} \cap F_i| = t > 0$ for some $i \in [r]$. Let C_x and C_y be the connected components of $G - F_i$ such that $x \in C_x$ and $y \in C_y$. Assume for a moment that $C_x = C_y$. Then there exits an x, y-path Q (in G) that lies completely in C_x. Clearly, Q contains no edge from F_i. On the other hand, as $t > 0$ there exists an edge $f = uv \in P_{x,y} \cap F_i$. Consider the closed walk between u and v consisting of the u, x-subpath of $P_{x,y}$, x, y-path Q, and y, v-subpath of $P_{x,y}$. By Lemma 2.1(ii), this closed walk contains an edge $f' \neq f$ such that $f\Theta f'$. Since $P_{x,y}$ is a geodesic, Lemma 2.1(i) implies that $f' \in Q$, a contradiction because from $f\Theta f'$ we know that $f' \in F_i$. It follows that $C_x \neq C_y$.

Let $f_1 = x_1y_1, \ldots, f_t = x_ty_t$ be the edges of $P_{x,y} \cap F_i$, indexed consecutively along $P_{x,y}$. Then any pair of vertices from the set $Z = \{x_1, \ldots, x_t\} \cup \{y_t\}$ is connected by a subpath of $P_{x,y}$ that contains an edge from F_i. (For instance, for the vertices x_t and y_t, the edge x_ty_t itself defines such a subpath.) Since each such subpath is a shortest path, using the argument from the previous paragraph it follows that the vertices from Z lie in pairwise different connected components of $G - F_i$. Consequently, by the definition of the quotient graph G/F_i, the shortest path $P_{x,y}$ induces a path of length t in G/F_i, so that $d_{G/F_i}(C_x, C_y) \leq t$. Assume now that $d_{G/F_i}(C_x, C_y) < t$ holds and let R be a shortest C_x, C_y-path in G/F_i. Then R can be naturally lifted into an x, y-path in G which contains less that t edges from F_i. Since this contradicts Lemma 2.1(iii), we conclude that $d_{G/F_i}(C_x, C_y) \geq t$ and consequently $d_{G/F_i}(C_x, C_y) = t$.

We have thus proved that if $\{x, y\} \in \binom{V_j}{2}$ and $|P_{x,y} \cap F_i| = t > 0$, then $d_{G/F_i}(C_x, C_y) = t$, where C_x and C_y are the connected components of $G - F_i$ with $x \in C_x$ and $y \in C_y$. Moreover, the same conclusion holds also in the case when $t = 0$. Hence if C and C' are connected components of $G - F_i$ with $|C \cap V_j| = a$ and $|C' \cap V_j| = b$, then the paths $P_{x,y}$, where $x, y \in V_j$, $x \in C$, $y \in C'$, contain $a \cdot b \cdot d_{G/F_i}(C, C')$ edges from F_i. Setting $w_i^{(j)}(C) = |C \cap V_j|$ for any connected component $C \in V(G/F_i)$ it follows that for any $j \in [k]$,

$$\sum_{\{x,y\}\in\binom{V_j}{2}} |E(P_{x,y}) \cap F_i| = W(G/F_i, w_i^{(j)})$$

and consequently

$$\sum_{j=1}^{k} \sum_{\{x,y\}\in\binom{V_j}{2}} |E(P_{x,y}) \cap F_i| = \sum_{j=1}^{k} W(G/F_i, w_i^{(j)}) \,.$$

Using (2) it follows that

$$\begin{aligned} W_{\mathcal{P}}(G) &= \sum_{i=1}^{r}\left(\sum_{j=1}^{k}\sum_{\{x,y\}\in\binom{V_j}{2}}|E(P_{x,y})\cap F_i|\right) \\ &= \sum_{i=1}^{r}\sum_{j=1}^{k}W(G/F_i, w_i^{(j)}) \end{aligned}$$

and we are done. □

Another concept that is very (but not completely) similar to the partition distance is the one of the modified Wiener index introduced in [10]. If G is a graph and $\{V_1, \ldots, V_k\}$ the partition of $V(G)$ into the orbits under the action of $\mathrm{Aut}(G)$, then the *modified Wiener index* of G is

$$|V(G)|\sum_{i=1}^{k}\frac{1}{|V_i|}\sum_{\{u,v\}\in\binom{V_i}{2}}d_G(u,v)\,.$$

Hence without the normalization terms, the modified Wiener index would be a special case of the partition distance. Nevertheless, in [7] it was demonstrated that also for the modified Wiener index a result parallel to Theorem 2.2 can be designed.

We say that a partition $\mathcal{E} = \{E_1, \ldots, E_t\}$ of $E(G)$ is *coarser than* $\mathcal{F} = \{F_1, \ldots, F_r\}$ if each set E_j is the union of one or more Θ^*-classes of G. Theorem 2.2 then generalizes as follows.

Theorem 2.3 *Let (G, w) be a connected weighted graph and let $\mathcal{P} = \{V_1, \ldots, V_k\}$ be a partition of $V(G)$. If $\{E_1, \ldots, E_r\}$ is a partition of $E(G)$ coarser than the Θ^*-partition, then*

$$W_{\mathcal{P}}(G,w) = \sum_{i=1}^{r}\sum_{j=1}^{k}W(G/E_i, w_i^{(j)})\,,$$

where $w_i^{(j)}(C) = \sum_{x\in C\cap V_j} w(x)$ for any $C \in V(G/E_i)$.

Since the proof of Theorem 2.3 proceed similarly as the proof of Theorem 2.2, we omit the details but point out that instead of Lemma 2.1(iii) one needs to apply the following result.

Lemma 2.4 [20, Lemma 3.2] *Let $\{E_1, \ldots, E_r\}$ be a partition of $E(G)$ coarser than the Θ^*-partition. Let C and C' be connected components of $G - E_i$, and let $x, y \in V(C)$, $x', y' \in V(C')$. If P_1 and P_2 are shortest x, x'- and y, y'-paths in G, respectively, then $|E(P_1) \cap E_i| = |E(P_2) \cap E_i|$.*

In the rest of the section we collect some consequences of Theorem 2.2. As already noted, if $|\mathcal{P}| = 1$, then $W_{\mathcal{P}}(G) = W(G)$. Hence Theorem 2.2 implies the following statement (rewritten here in the present notation) which is the main result of [19].

Corollary 2.5 [19, Theorem 2.1] *If $\{F_1, \ldots, F_r\}$ is the Θ^*-partition of a connected graph G, then*

$$W(G) = \sum_{i=1}^{r} W(G/F_i, w_i)\,,$$

where $w_i(C) = |C|$ for any $C \in V(G/F_i)$.

Combining (1) with Theorem 2.2 and Corollary 2.5 we get:

Corollary 2.6 *Let G be a connected graph and let $\mathcal{P} = \{V_1, \ldots, V_k\}$ be a partition of $V(G)$. If $\{F_1, \ldots, F_r\}$ is the Θ^*-partition of $E(G)$, then*

$$W_{\overline{\mathcal{P}}}(G) = \sum_{i=1}^{r} \left[W(G/F_i, w_i) - \sum_{j=1}^{k} W(G/F_i, w_i^{(j)}) \right]\,,$$

where $w_i(C) = |C|$ and $w_i^{(j)}(C) = |C \cap V_j|$ for any $C \in V(G/F_i)$.

Another direct consequence of Theorem 2.2 is the following result which is in turn a generalization of [16, Theorem 5.1] from graphs isometrically embeddable into hypercubes to general graphs.

Corollary 2.7 *If G is a connected graph, X the set of vertices of G of degree ℓ, and $\{F_1, \ldots, F_r\}$ the Θ^*-partition of $E(G)$, then*

$$TW_\ell(G) = \sum_{i=1}^{r} W(G/F_i, w_i)\,,$$

where $w_i(C) = |C \cap X|$ for any $C \in V(G/F_i)$.

Proof. Let $\mathcal{P} = \{V_1, \ldots, V_k\}$ be the partition of $V(G)$ in which V_1 consists of all the vertices of degree ℓ, while each of the remaining parts of the partition is of order 1. Then (in the notation of Theorem 2.2) $W(G/F_i, w_i^{(j)}) = 0$ for any $i \in [r]$ and for any $j \in [k] \setminus \{1\}$. Hence the result. □

For results of a similar nature than Corollary 2.7 and are important in chemical graph theory we refer to the recent survey [21], where the investigation done in the present paper has been indicated [21, Section 4.5], also see [1].

3 Bounds on the partition distance of trees

In this section we apply the results of the previous section to derive bounds on the partition distance of trees.

Recall that the center of a graph G is the set of its vertices that minimize the eccentricity of G. It is well-known that the center of a tree can be obtained by iteratively removing the set of its leaves. Consequently, the center of a tree consists either of a single vertex or of two adjacent vertices. In the first case the tree is called *centered* and in the latter case it is *bicentered*.

A *subdivided star* is a tree obtained from a star by subdividing its edges (not necessarily all of them). A subdivided star is *balanced* if all the edges of a star are subdivided by the same number of vertices (possibly zero). Similarly, a *balanced subdivided double star* is obtained from P_2 by attaching to both of its vertices the same number of paths of the same length. Note that balanced subdivided double stars are bicentered tree. Note also that paths of odd order are balanced subdivided stars while paths of even order are balanced subdivided double stars.

Theorem 3.1 *Let T be a tree of order $n \geq 3$ and radius r, and let $\mathcal{P} = \{V_1, \ldots, V_k\}$ be a partition of $V(T)$.*

(i) If T is a centered tree, then

$$W_{\mathcal{P}}(T) \leq \left(\frac{r}{n-1}\right)(n-r-1) \sum_{\substack{i=1 \\ |V_i|\geq 2}}^{k} |V_i|^2 \,,$$

where the equality holds if and only if T is a balanced subdivided star, V_1 contains the pendant vertices of T, and $|V_i| = 1$ for $i \geq 2$.

(ii) If T is a bicentered tree, then

$$W_{\mathcal{P}}(T) \leq \left(\frac{1}{4} + \frac{(n-r-1)(r-1)}{n-2}\right) \sum_{\substack{i=1 \\ |V_i|\geq 2}}^{k} |V_i|^2 \,,$$

where the equality holds if and only if T is a balanced subdivided double star, V_1 contains the pendant vertices of T, and $|V_i| = 1$ for $i \geq 2$.

Proof. Suppose first that $k = 1$. Then because $1 \leq r \leq n/2$ easy computations show that both asserted upper bounds are of the form $n^3/2 + O(n^2)$. Among the n-vertex graphs (and hence among the n-vertex trees) the Wiener index is maximized on paths fow which $W(P_n) = (n^3 - n)/6$ holds [6]. It now readily follows that the asserted inequality holds for $k = 1$. In the rest we thus assume that $k \geq 2$ and set $p_\ell = |V_\ell|$, $\ell \in [k]$.

Assume first that T is a centered tree with radius r and with v in its center. Let $N_i(v) = \{x \in V(T) :\ d(x, v) = i\}$ and set $n_i = |N_i(v)|$, $i \in [r]$. If E_i is the set of edges between $N_{i-1}(v)$ and $N_i(v)$, then $\mathcal{E} = \{E_1, \ldots, E_r\}$ is a partition of $E(T)$. Clearly, $\mathcal{E}$ is a partition coarser than the Θ^*-partition because it is well-known (and easy to see) that the parts of the latter are single edges. Hence Theorem 2.3 can be applied to T, $\mathcal{P}$, and $\mathcal{E}$. The quotient graph T/E_i is the star K_{1,n_i}, its center vertex corresponding to the component of $T - E_i$ containing v. Let p_{ij}^{ℓ}, $i \in [r]$, $j \in [n_i + 1]$, $\ell \in [k]$, be the number of vertices from V_ℓ that lie in the j^{th} connected component of $T - E_i$. In particular, p_{i1}^{ℓ} is the number of vertices from V_ℓ in the connected component of $T - E_i$ containing v. Setting

$$W_{\mathcal{P}}^{\ell}(T) = 2\sum_{i=1}^{r} \sum_{2\le j<j'\le n_i+1} p_{ij}^{\ell} p_{ij'}^{\ell} + \sum_{i=1}^{r} p_{i1}^{\ell}\left(p_\ell - p_{i1}^{\ell}\right), \tag{3}$$

we infer from Theorem 2.3 that

$$W_{\mathcal{P}}(T) = \sum_{\ell=1}^{k} W_{\mathcal{P}}^{\ell}(T)\,. \tag{4}$$

Note that if $p_\ell = 1$, then $W_{\mathcal{P}}^{\ell}(T) = 0$. Hence, in the following we may assume that $p_\ell \ge 2$.

Clearly, (3) will be largest when $p_{ij}^{\ell} = p_{ij'}^{\ell} = \frac{p_\ell - p_{i1}^{\ell}}{n_i}$ holds for all $j \neq j'$. Therefore,

$$\begin{aligned} W_{\mathcal{P}}^{\ell}(T) &= 2\sum_{i=1}^{r} \sum_{2\le j<j'\le n_i+1} p_{ij}^{\ell} p_{ij'}^{\ell} + \sum_{i=1}^{r} p_{i1}^{\ell}\left(p_\ell - p_{i1}^{\ell}\right) \\ &\le 2\sum_{i=1}^{r} \binom{n_i}{2}\left(\frac{p_\ell - p_{i1}^{\ell}}{n_i}\right)^2 + \sum_{i=1}^{r} p_{i1}^{\ell}\left(p_\ell - p_{i1}^{\ell}\right) \\ &= \sum_{i=1}^{r} \left(p_\ell - p_{i1}^{\ell}\right)\left(p_\ell - \frac{p_\ell - p_{i1}^{\ell}}{n_i}\right) \\ &= p_\ell \sum_{i=1}^{r} \left(p_\ell - p_{i1}^{\ell}\right) - \sum_{i=1}^{r} \frac{(p_\ell - p_{i1}^{\ell})^2}{n_i}\,. \end{aligned} \tag{5}$$

Using the weighted arithmetic-harmonic mean (cf. [23, p. 21]), and having in mind that

$\sum_{i=1}^r n_i = n-1$, we can continue as follows:

$$
\begin{aligned}
W_{\mathcal{P}}^\ell(T) &\le p_\ell \sum_{i=1}^r \left(p_\ell - p_{i1}^\ell\right) - \sum_{i=1}^r \frac{(p_\ell - p_{i1}^\ell)^2}{n_i} \\
&\le p_\ell \sum_{i=1}^r (p_\ell - p_{i1}^\ell) - \frac{\left(\sum_{i=1}^r (p_\ell - p_{i1}^\ell)\right)^2}{n-1} \qquad (6) \\
&= \left(\sum_{i=1}^r (p_\ell - p_{i1}^\ell)\right)\left(p_\ell - \frac{p_\ell \cdot r}{n-1} + \frac{\sum_{i=1}^r p_{i1}^\ell}{n-1}\right) \\
&= \left(p_\ell \cdot r - \sum_{i=1}^r p_{i1}^\ell\right)\left(p_\ell\left(1 - \frac{r}{n-1}\right) + \frac{\sum_{i=1}^r p_{i1}^\ell}{n-1}\right) \\
&= p_\ell^2 \cdot r\left(1 - \frac{r}{n-1}\right) + \left(\sum_{i=1}^r p_{i1}^\ell\right)\left(p_\ell\left(\frac{2r}{n-1} - 1\right) - \frac{\sum_{i=1}^r p_{i1}^\ell}{n-1}\right). \qquad (7)
\end{aligned}
$$

Since $n \ge 2r+1$, the second term of (7), that is,

$$
\left(\sum_{i=1}^r p_{i1}^\ell\right)\left(p_\ell\left(\frac{2r}{n-1} - 1\right) - \frac{\sum_{i=1}^r p_{i1}^\ell}{n-1}\right), \qquad (8)
$$

is non-positive. Therefore, for any fixed ℓ, we have:

$$
W_{\mathcal{P}}^\ell(T) \le p_\ell^2 \cdot r\left(1 - \frac{r}{n-1}\right) = p_\ell^2 (n-r-1)\frac{r}{n-1}. \qquad (9)
$$

The claimed inequality for centered trees now follows immediately.

The asserted inequality for centered trees now follows by combining (9) with (4).

In the second case assume that T is a bicentered tree of radius r. Let u and v be the central vertices of T, set $e = uv$, and let $N_i(e) = \{x \in V(T) : d(x,e) = i\}$, $i \in \{0,1,\ldots,r-1\}$. Let E_i be the set of edges between $N_{i-1}(e)$ and $N_i(e)$ and set $n_i = |N_i(e)|$. Then $\mathcal{E} = \{E_0 = \{e\}, E_1, \ldots, E_{r-1}\}$ is a partition of $E(T)$ coarser than the Θ^*-partition. Therefore, using the notation of the first case,

$$
W_{\mathcal{P}}^\ell(T) = p_{01}^\ell \cdot p_{02}^\ell + 2\sum_{i=1}^{r-1} \sum_{2\le j<j'\le n_i+1} p_{ij}^\ell \cdot p_{ij'}^\ell + \sum_{i=1}^{r-1} p_{i1}^\ell \left(p_\ell - p_{i1}^\ell\right), \qquad (10)
$$

where p_{0j}^ℓ, $j \in [2]$, are the weights of the vertices in the quotient graph T/E_0. Applying the same arguments as for centered trees we get:

$$
W_{\mathcal{P}}^\ell(T) \le \frac{p_\ell^2}{4} + \frac{p_\ell^2 (n-r-1)(r-1)}{n-2} = \left(\frac{1}{4} + \frac{(n-r-1)(r-1)}{n-2}\right) p_\ell^2,
$$

hence the inequality of the theorem follows also for bicentered trees.

It remains to prove the equality part of the theorem. Let us prove it for centered trees, the arguments for bicentered trees are parallel. So let T be a centered tree with the center v. Then the equality holds if and only if for any $\ell \in [k]$, the inequalities (5), (6) and (9) are equalities. Now fix ℓ. Then in the equality case, for any $i \in [r]$ and any j, $2 \leq j \leq n_i + 1$,

$$p_{ij}^{\ell} = (p_\ell - p_{i1}^{\ell})/n_i, \tag{11}$$

$$\frac{p_\ell - p_{11}^{\ell}}{n_1} = \frac{p_\ell - p_{21}^{\ell}}{n_2} = \cdots = \frac{p_\ell - p_{r1}^{\ell}}{n_r}, \tag{12}$$

and

$$\sum_{i=1}^{r} p_{i1}^{\ell} = 0 \tag{13}$$

or

$$p_\ell \left(2r/(n-1) - 1\right) - \sum_{i=1}^{r} p_{i1}^{\ell}/(n-1) = 0 \tag{14}$$

For any $i \in [r]$ and any j, $2 \leq j \leq n_i+1$, the equality $p_{ij}^{\ell} = (p_\ell - p_{i1}^{\ell})/n_i$ demonstrates that the weights of the leaves in the quotient graphs T/E_i are the same. We now claim $n_1 = \cdots = n_r$ and $p_{11}^{\ell} = \cdots = p_{r1}^{\ell}$. First, we prove $n_1 \leq \cdots \leq n_r$. Assume on the contrary that there exists $1 \leq t \leq r-1$ such that $n_t > n_{t+1}$. Hence $N_t(v)$ contains at least one pendant vertex, say u. Since $k \geq 2$, we may assume without loss of generality that $u \notin V_1$. Note that the expression on the right-hand side of (11) is independent from j, and since $p_{tj'}^{1} = 0$, where j' corresponds to the components $\{u\}$ of $G - E_t$, we infer that $w \notin V_1$ for any vertex w with $d(w,v) \geq t+1$. It follows that $p_1 - p_{t+1,1}^{1} = 0$, and from (12) we find out that $p_1 = p_{11}^{1} = 1$ which is not possible.

We have thus proved that $n_1 \leq \cdots \leq n_r$. It then follows from (12) that $p_{11}^{\ell} \geq \cdots \geq p_{r1}^{\ell}$. Since on the other hand we clearly have $p_{11}^{\ell} \leq \cdots \leq p_{r1}^{\ell}$, we conclude that $p_{11}^{\ell} = \cdots = p_{r1}^{\ell}$. Using (12) again we also get that $n_1 = \cdots = n_r$.

It implies that the central vertex of the star quotient graph has constant weight for each i. Since $p_\ell \geq 2$, it follows from the above that only pendant vertices at distance r from v and the vertex v can belong to V_ℓ. If $v \in V_\ell$, then $\sum_{i=1}^{r} p_{i1}^{\ell} = r$ and must $p_\ell\left(2r/(n-1) - 1\right) - r/(n-1) = 0$, that is, $n = 2r + 1 - r/p_\ell$. On the other hand, T is a centered tree and then $n \geq 2r+1$ which is not possible. Hence, $\sum_{i=1}^{r} p_{i1}^{\ell} = 0$ must be true and just pendants vertices are in V_ℓ that are all at distance r from the root, and since $n_1 = \cdots = n_r$, we conclude that T is a balanced subdivided star. As already mentioned, using similar arguments the equality case follows for bicentered trees. $\square$

With respect to Theorem 3.1 we mention that for each fixed pair (n, r), $n \leq 20$, trees that maximize the Wiener index among the n-vertex trees of radius r were found by computer in [15].

The next result on the terminal Wiener index follow immediately from Theorem 3.1 by partitioning $V(T)$ into the class of leaves and singletons.

Corollary 3.2 *Let T be a tree of order $n \geq 3$, radius r, and with p pendant vertices.*
(i) If T is a centered tree, then

$$TW(T) \leq \frac{p^2 r(n-r-1)}{n-1},$$

where the equality holds if and only if T is a balanced subdivided star.
(ii) If T is bicentered tree, then

$$TW(T) \leq p^2 \left(\frac{1}{4} + \frac{(n-r-1)(r-1)}{n-2} \right),$$

where the equality holds if and only if T is a balanced subdivided double star graph.

Although the following results has a simple direct proof, we state it here as a consequence of Theorem 3.1. To do so, one only has to observe that $r(n-r-1)/(n-1) \leq (n-1)/4$ holds for any possible r in the case of center trees, and similarly for bicentered trees.

Corollary 3.3 *If T is a tree of order $n \geq 3$ and $\mathcal{P} = \{V_1, \ldots, V_k\}$ is a partition of $V(T)$, then*

$$W_{\mathcal{P}}(T) \leq \frac{n-1}{4} \sum_{\substack{i=1 \\ |V_i| \geq 2}}^{k} |V_i|^2 .$$

Moreover, equality holds if and only if T is a path, V_1 contains the two pendant vertices of T, and $|V_i| = 1$ for $i \geq 2$.

Corollary 3.3 in turn implies the following result on the generalized terminal Wiener index.

Corollary 3.4 *If T is a tree of order $n \geq 3$ and with d_k vertices of degree $k \geq 1$, then*

$$TW_k(T) \leq \frac{d_k^2}{4}(n-1).$$

In particular, if p is the number of pendant vertices of T, then

$$TW(T) \leq \frac{p^2}{4}(n-1),$$

where the equality holds if and only if $T = P_n$.

4 Concluding remarks

As mentioned in the introduction, the generalized terminal Wiener index [16] and the terminal Wiener index [11] are special cases of the partition distance. We point out that the (generalized) terminal Wiener index can not be defined in terms of $W_{\overline{\mathcal{P}}}(G)$ only. For instance, if T is a tree on at least three vertices, then it has at least two leaves. In order to define $W_{\overline{\mathcal{P}}}(T)$, all the leaves would have to be in pairwise different parts of $\mathcal{P}$, but then $W_{\overline{\mathcal{P}}}(T)$ would take into the account also some distances between leaves and non-leaves. This example shows that the duality of the partition distance and the colored distance must be taken with care.

If $X \subseteq V(G)$, then the *relative Wiener index* $W_X(G)$ (introduced in [2] and mentioned in the introduction) is defined is the sum of the distances between all pairs of vertices form X. In [8] the *k-diameter* $d_k(G)$ of a graph G was introduced as $\max\{W_X(G) : |X| = k\}$, that is, as the maximum over all partition distances with all but one parts being singletons, while the remaining part is of size k. Note that $d_2(G) = \mathrm{diam}(G)$ and $d_{|V(G)|}(G) = W(G)$. In [8] the 3-diameter has been considered, the maximum size of a graph with given order and 3-diameter was determined. No further developments on the k-diameter are known, except that based on it, the (k, ℓ)-eccentricity has been introduced in [13]. It would certainly be interesting to further investigate the k-diameter, in particular to obtain general (optimal) bounds on it as well as to classify corresponding extremal graphs.

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