Wiener Index Versus Maximum Degree in Trees

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Abstract. The Wiener index of a graph is the sum of all pairwise distances of vertices of the graph. In this paper we characterize the trees which minimize the Wiener index among all trees of given order and maximum degree and the trees which maximize the Wiener index among all trees of given order that have only vertices of two different degrees.

Keywords. Tree; Wiener Index; Average Distance; Degree; Valency

1 Terminology and Introduction

All graphs in this paper will be finite, simple and undirected and we will use standard graph-theoretical terminology. For a graph $G = (V(G), E(G))$, the order will be denoted by $n(G) = |V(G)|$ and the neighbourhood of a vertex $v \in V(G)$ will be denoted by $N_G(v)$. The degree $d_G(v)$ of a vertex $v \in V(G)$ in the graph G is $|N_G(v)|$. A vertex of degree one is an endvertex. The maximum degree $\max_{v \in V(G)} d_G(v)$ of a graph G is denoted by $\Delta(G)$. The subgraph of G induced by a set $X \subseteq V(G)$ is denoted by $G[X]$.

The *distance* $d_G(u, v)$ between two vertices $u, v \in V(G)$ in the graph G is the minimum number of edges on a path in G from u to v or ∞ if no such path exists. The *distance sum*

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$\sigma_G(u)$ *of* G *with respect to a vertex* $u \in V(G)$ is defined as $\sigma_G(u) = \sum_{v \in V(G)} d_G(u,v)$ and the *distance sum* $\sigma(G)$ *of* G or *Wiener index* of G is defined as

$$\sigma(G) = \frac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} d_G(u,v) = \frac{1}{2} \sum_{u \in V(G)} \sigma_G(u).$$

The *average distance* $\bar{d}(G)$ of a graph G is $\frac{\sigma(G)}{\binom{n(G)}{2}}$.

The Wiener index and the average distance rank among those graph-theoretical parameters that are of most interest to other sciences. In fact, it was the chemist H. Wiener who in 1947 proposed σ in [19] and [20] as a measure for the degree of molecular branching which seems to be related to many physical and chemical properties of molecules. There are numerous publications on the average distance $\bar{d}$ and the Wiener index σ both in mathematical and chemical journals. See for example [1], [2], [7], [8], [9], [10], [12], [16], [18], and [21] for theoretical and [3], [6], [11] and [17] for algorithmical and computational aspects. A recent and very comprehensive survey about the Wiener index is [5].

Chemists are often interested in the Wiener index of certain trees which represent molecular structures. Entringer, Jackson and Snyder [9] proved that among all trees of a given order n the Wiener index is maximized by the path P_n and minimized by the star $K_{1,n-1}$. Since every atom has a certain *valency*, chemists are also often interested in graphs with restricted degrees=valencies. It is therefore not a really satisfactory answer to say that stars minimize the Wiener index, since their maximum degree grows arbitrarily. This motivates the central problem that we consider in this paper.

Problem 1.1 *What trees minimize the Wiener index among all trees of given order* n *and maximum degree at most* Δ*?*

Clearly Problem 1.1 is only interesting if the maximum degree is at least 3. We will settle Problem 1.1 in section two. Our answer to Problem 1.1 will lead us to trees which (with one possible exception) have only vertices of degrees 1 and Δ. For these we solve the following opposite problem in section three.

Problem 1.2 *What trees maximize the Wiener index among all trees of given order* n *whose vertices are either endvertices or of maximum degree* Δ*?*

Once again, this question is only interesting if the maximum degree is at least 3.

2 Trees with minimum Wiener Index

We define a class of trees which will be the extremal trees for Problem 1.1.

Definition 2.1 *Let $\Delta \geq 3$ and $R \in \{\Delta - 1, \Delta\}$. For every n the family $\mathcal{T}(R, \Delta)$ of trees has a unique member T of order n up to isomorphism which we now define together with a natural plane embedding.*

Let $M_0(R, \Delta) = 1$ and $M_1(R, \Delta) = 1 + R$, and let $M_k(R, \Delta) = 1 + R + R(\Delta - 1) + ... + R(\Delta - 1)^{k-1}$ for $k \geq 2$. Let

$$M_k(R, \Delta) \leq n < M_{k+1}(R, \Delta) \tag{1}$$

for some $k \geq 0$. Let $n - M_k(R, \Delta) = m(\Delta - 1) + r$ for some $0 \leq r < \Delta - 1$, if $k \geq 1$; and $r = n - 1$ for $k = 0$. Let T be the tree of order n embedded in the plane such that (see Figure 1)

(i) all vertices of T lie on some line $\mathbf{R} \times \{i\}$ for $0 \leq i \leq k + 1$,

(ii) there is a unique vertex on line $\mathbf{R} \times \{0\}$ which has exactly $\min\{n - 1, R\}$ neighbours that lie on line $\mathbf{R} \times \{1\}$,

(iii) for $1 \leq j \leq k - 1$ every vertex on line $\mathbf{R} \times \{j\}$ has a unique neighbour on line $\mathbf{R} \times \{j - 1\}$ and $\Delta - 1$ neighbours on line $\mathbf{R} \times \{j + 1\}$,

(iv) if $v_1, v_2, ..., v_{m+1}$ are the $m + 1$ leftmost vertices on line $\mathbf{R} \times \{k\}$ such that v_i lies left of v_j for $i < j$, then each of $v_1, v_2, ..., v_m$ has $\Delta - 1$ neighbours on line $\mathbf{R} \times \{k + 1\}$ and v_{m+1} has r neighbours on line $\mathbf{R} \times \{k + 1\}$.

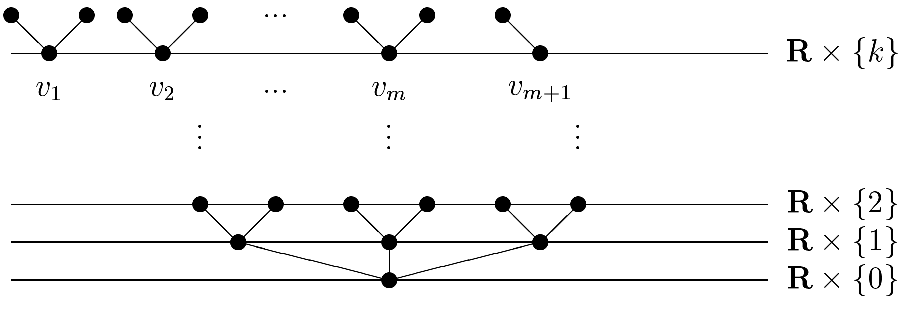

Figure 1

Our main result in this section is the following.

Theorem 2.2 *Let T be a tree of order n and maximum degree at most Δ ($\Delta \geq 3$). Then $\sigma(T) \leq \sigma(T')$ for all trees T' of order n and maximum degree at most Δ*

In fact, Theorem 2.2 has been verified by a computer search for all chemical trees, i.e. trees of maximum degree 4, of order up to 21 in [15]. The trees in $\mathcal{T}(4,4)$ represent alkanes which are called *dendrimers* and whose Wiener index has been studied in [4] and [13].

In the proof of Theorem 2.2 we may assume $n > 1+\Delta$ by [9], i.e. $k \geq 1$ in (1). In the proof of Theorem 2.2 we will consider the *centroid* of a tree. For some tree T and a vertex $v \in V(T)$, a *branch* of T at v is a maximal subtree of T that contains v as an endvertex. The *weight* $bw(B)$ of a branch B is the number of edges in B and the *branchweight* $bw(v)$ of $v \in V(T)$ is the maximum weight of a branch at v. The *centroid* $C(T)$ of a tree T is the set of vertices of T of minimum branchweight. We need the following properties of the centroid of a tree.

Theorem 2.3 (Jordan [14]) *If T is a tree, then either $C(T) = \{c\}$ and $bw(c) \leq \frac{n-1}{2}$ or $C(T) = \{c_1, c_2\}$, $c_1c_2 \in E(T)$ and $bw(c_1) = bw(c_2) = \frac{n}{2}$.*

Furthermore, we need the following property of the trees in $\mathcal{T}(R,\Delta)$.

Lemma 2.4 *Let $T \in \mathcal{T}(R,\Delta)$ have order n and let $M_k(R,\Delta) < n < M_{k+1}(R,\Delta)$ for some $k \geq 1$. Let T' arise from the tree T_0 in $\mathcal{T}(R,\Delta)$ of order $M_k(R,\Delta)$ by attaching $n - M_k(R,\Delta)$ endvertices that lie on the line $\mathbf{R} \times \{k+1\}$ to the vertices of T_0 that lie on the line $\mathbf{R} \times \{k\}$.*

Then either $\sigma(T) < \sigma(T')$ or T and T' are isomorphic.

Proof: We assume that T' is such that it has minimum distance sum among all trees that satisfy the assumption of Lemma 2.4 and show that T and T' are isomorphic.

Let $v \in V(T_0) \subseteq V(T')$. The vertex v lies on line $\mathbf{R} \times \{i\}$ for some $0 \leq i \leq k$. Let T_v denote the maximal subtree of T' that contains v and has only vertices on lines $\mathbf{R} \times \{j\}$ for $j \geq i$. We say that T_v is *full* (*empty*) if all vertices of T_v on line $\mathbf{R} \times \{k\}$ have degree Δ (1, respectively).

Claim. Let $v \in V(T_0) \subseteq V(T')$ lie on line $\mathbf{R} \times \{i\}$ for some $0 \leq i \leq k-1$. Let $v_1, v_2, ..., v_l$ be the neighbours of v on line $\mathbf{R} \times \{i+1\}$. Then at most one of the trees $T_{v_1}, T_{v_2}, ..., T_{v_l}$ is neither full nor empty.

Proof of the Claim: We assume for contradiction that the claim does not hold for the vertex $v \in V(T_0) \subseteq V(T')$ that lies on line $\mathbf{R} \times \{i\}$ for some $0 \leq i \leq k-1$ and that i is maximum under this condition, i.e. the claim holds for all vertices on lines $\mathbf{R} \times \{j\}$ for $j > i$. We may assume furthermore that T_{v_1} and T_{v_2} are neither full nor empty and that T_{v_1} has at least as many vertices on line $\mathbf{R} \times \{k+1\}$ as T_{v_2}. Let V_i denote the set of vertices of T_{v_i} on line $\mathbf{R} \times \{k+1\}$ for $i = 1, 2$.

Let x and y be two vertices in $V(T_{v_1})$ or in $V(T_{v_2})$ that lie both on line $\mathbf{R} \times \{j\}$ for some $i+2 \leq j \leq k$. If T_x is full (empty) and T_y is not full (empty), then we assume that x lies left (right) of y. Thus, for $\nu = 1, 2$ there is at most one vertex in $V(T_{v_\nu})$ on line $\mathbf{R} \times \{k\}$ of degree $\neq 1, \Delta$ and for two vertices $x, y \in V(T_{v_\nu})$ on line $\mathbf{R} \times \{k\}$ we have $d_T(x) \geq d_T(y)$, if x lies left of y.

Let V_ν denote the vertices of T_{v_ν} on line $\mathbf{R} \times \{k+1\}$ for $\nu = 1, 2$ and let

$$p = \min\{(\Delta - 1)^{k-i} - |V_1|, |V_2|\}.$$

Since T_{v_1} and T_{v_2} are neither full nor empty, we have $1 \leq |V_2| \leq |V_1| < (\Delta - 1)^{k-i}$ and hence $p \geq 1$. For $q = \lceil \frac{p}{\Delta - 1} \rceil$ let $y_1, y_2, \ldots, y_q$ (and $z_1, z_2, \ldots, z_q$, respectively) be the rightmost (leftmost, respectively) q vertices in $V(T_{v_1})$ ($V(T_{v_2})$) on line $\mathbf{R} \times \{k\}$. Furthermore, let $x_1, x_2, \ldots, x_p$ be the p leftmost vertices in V_2 and let T'' be the tree with vertex set $V(T')$ and edge set (see Figure 2)

$$(E(T') \setminus \{x_j z_{\lceil j/(\Delta-1) \rceil} \mid 1 \leq j \leq p\}) \cup \{x_j y_{\lceil j/(\Delta-1) \rceil} \mid 1 \leq j \leq p\}.$$

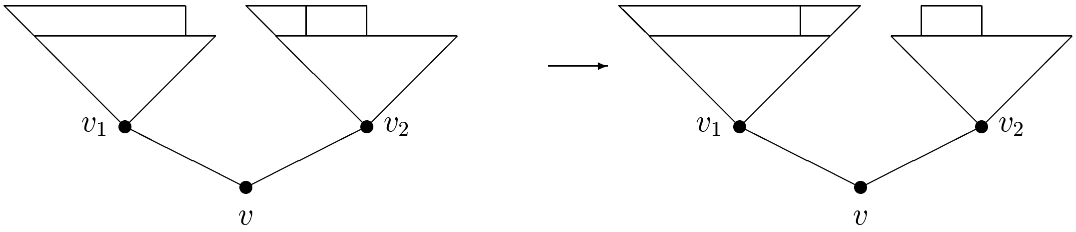

Figure 2

Going from T' to T'' the sum of the distances between all pairs of vertices in $V(T) \setminus \{x_1, x_2, \ldots, x_p\}$ and for every $1 \leq \nu \leq p$ the sum of the distances from x_ν to all vertices in $(V(T) \setminus (V_1 \cup V_2)) \cup \{x_1, x_2, \ldots, x_p\}$ remain unchanged. This implies that

$$\sigma(T') - \sigma(T'') = \sum_{\substack{x \in \{x_1, x_2, \ldots, x_p\} \\ y \in V_1 \cup V_2 \setminus \{x_1, x_2, \ldots, x_p\}}} (d_{T'}(x,y) - d_{T''}(x,y)).$$

The tree $T''[V(T_{v_1}) \cup \{x_1, x_2, \ldots, x_p\}]$ contains a tree $T^*_{v_2} \cong T_{v_2}$ as a subgraph such that $\{x_1, x_2, \ldots, x_p\} \subseteq V(T^*_{v_2})$. Let $V_1^* = V_1 \setminus V(T^*_{v_2})$. Note that $V_1^* \neq \emptyset$ and that $V_1^* = V_1$ if $p = |V_2|$. Thus,

$$\sum_{\substack{x \in \{x_1, x_2, \ldots, x_p\} \\ y \in (V_1 \setminus V_1^*) \cup V_2 \setminus \{x_1, x_2, \ldots, x_p\}}} (d_{T'}(x,y) - d_{T''}(x,y)) = 0$$

and

$$\begin{aligned} \sigma(T') - \sigma(T'') &= \sum_{\substack{x \in \{x_1, x_2, \ldots, x_p\} \\ y \in V_1^*}} (d_{T'}(x,y) - d_{T''}(x,y)) \\ &\geq \sum_{\substack{x \in \{x_1, x_2, \ldots, x_p\} \\ y \in V_1^*}} (2(k+1-i) - 2(k-i)) > 0 \end{aligned}$$

which is a contradiction to the choice of T' and the claim is proved.
□

If we now embed T' in the plane in the same way as T_{v_1} and T_{v_2} at the beginning of the proof of the claim, then it is easy to see that T and T' are isomorphic and the proof of Lemma 2.4 is complete.
□

Our next theorem will imply Theorem 2.2. We need some more terminology. Let T be some tree and let u, v and w be vertices in T. We say that v separates u and w, if v lies on the unique path in T from u to w. Let v be some vertex of T. If $C(T) \neq \{v\}$, then let T_v denote the subtree of T that contains v and all vertices u of T such that v separates u from all vertices in the centroid $C(T)$ of T. If $C(T) = \{v\}$, then let $T_v = T$.

Theorem 2.5 *Let T be a tree of order n and maximum degree at most Δ ($\Delta \geq 3$). Let $\sigma(T) \leq \sigma(T')$ for all trees T' of order n and maximum degree at most Δ.*
Then $T_v \in \mathcal{T}(\Delta - 1, \Delta)$ if $C(T) \neq \{v\}$ and $T_v \in \mathcal{T}(\Delta, \Delta)$ if $C(T) = \{v\}$ for all $v \in V(T)$.

Proof: If $n \leq 1 + \Delta$, then Theorem 2.5 follows from the cited result of [9]. Hence we may assume $n > 1 + \Delta$ and $k \geq 1$ in (1). We will prove Theorem 2.5 by induction on the maximum distance $h(T_v)$ of v to an endvertex in T_v. If $C(T) \neq \{v\}$, then let $R = \Delta - 1$ and if $C(T) = \{v\}$, then let $R = \Delta$. If $h(T_v) \in \{0, 1\}$, then the result is trivial. Now let $h(T_v) \geq 2$.

Claim. Let $P : v = x_1x_2...x_\nu$ be a path in T_v such that $x_1 \in C(T)$, $x_2 \notin C(T)$. Then $d_T(x_j) = \Delta$ for all $1 \leq j \leq \nu - 2$.

Proof of the Claim: We assume that $d_T(x_j) < \Delta$ for some $1 \leq j \leq \nu - 2$. Let $V_{j+2} = V(T_{x_{j+2}})$, $V_{j+1} = V(T_{x_{j+1}}) \setminus V_{j+2}$ and $V_j = V(T) \setminus (V_{j+1} \cup V_{j+2})$. By the definition of the centroid and the tree T_v we have $|V_j| > |V_{j+1}|$. Let T' be the tree with vertex set $V(T)$ and edge set $(E(T) \setminus \{x_{j+1}x_{j+2}\}) \cup \{x_jx_{j+2}\}$. We have $\sigma(T) - \sigma(T') = |V_{j+2}|(|V_j| - |V_{j+1}|) > 0$ which is a contradiction. This completes the proof of the claim.
□

Case 1. There exist two endvertices l_1 and l_2 in T_v such that $d_T(v, l_2) \geq d_T(v, l_1) + 2$.

Let l_1 (l_2) have minimum (maximum) distance d_1 (d_2) from v among all endvertices in T_v. By induction, the vertices l_1 and l_2 cannot lie in a proper subtree of T_v that does not contain v. Therefore, let v_1 and v_2 be two different neighbours of v in T_v such that v_i separates l_i and v for $i = 1, 2$. By induction, $T_{v_i} \in \mathcal{T}(\Delta - 1, \Delta)$ for $i = 1, 2$. Let u be the neighbour of v_2 that separates l_2 and v_2. We assume that T_{v_1} and T_{v_2} are embedded in the plane similarly as in Definition 2.1 such that v_1 and v_2 lie on the line $\mathbf{R} \times \{0\}$, u lies on the line $\mathbf{R} \times \{1\}$, l_1 lies on the line $\mathbf{R} \times \{d_1 - 1\}$, l_2 lies on the line $\mathbf{R} \times \{d_2 - 1\}$ and the vertices in $V(T_{v_1})$ and $V(T_{v_2})$ lie on the lines $\mathbf{R} \times \{j\}$ for $0 \leq j \leq d_1$ and $0 \leq j \leq d_2 - 1$, respectively. Without loss of generality let l_2 be the vertex of T_{v_2} lying rightmost on line $\mathbf{R} \times \{d_2 - 1\}$.

Let $V_3 = V(T_{v_2}) \setminus V(T_u)$. By the definition of the centroid and of the tree T_v, we have that

$$|V(T_u)| + |V_3| = |V(T_{v_2})| \leq bw(v) \leq bw(v_2) = |V(T) \setminus V(T_{v_2})|.$$

First, we assume that $|V(T_{v_1})| < |V(T_u)|$. This implies that $|V_3| < |V(T) \setminus (V(T_{v_1}) \cup V(T_{v_2}))|$. Let T' be the tree with vertex set $V(T)$ and edge set $E(T') = (E(T) \setminus \{v_2u, vv_1\}) \cup \{uv, v_1v_2\}$. We obtain

$$\sigma(T) - \sigma(T') = (|V(T_u)| - |V(T_{v_1})|) \cdot (|V(T) \setminus (V(T_{v_1}) \cup V(T_{v_2}))| - |V_3|) > 0$$

which is a contradiction. Hence $|V(T_{v_1})| \geq |V(T_u)|$. Since $T_{v_1}, T_{v_2} \in \mathcal{T}'(\Delta - 1, \Delta)$, we have that

$$1 + \sum_{i=0}^{d_2-3} (\Delta - 1)^i \leq |V(T_u)| \leq |V(T_{v_1})| < \sum_{i=0}^{d_1} (\Delta - 1)^i$$

which implies that $d_1 > d_2 - 3$. Since $d_1 \leq d_2 - 2$, we obtain $d = d_1 = d_2 - 2$.

Analogously as in the proof of Lemma 2.4 we want to construct a new tree T' such that $\sigma(T) > \sigma(T')$. For $i = 1, 2$ let V_i be the set of vertices of T_{v_i} on line $\mathbf{R} \times \{d - 1 + i\}$. Note, that $T_{v_1} - V_1 \cong T_u - V_2$. By the choice of l_2, we obtain

$$V_2 \subseteq V(T_u), \ |V_1| \geq |V_2|, \ \text{ and } \ |V_3| \leq 1 + \sum_{i=0}^{d-1} (\Delta - 2)(\Delta - 1)^i.$$

Let $p = \min\{(\Delta - 1)^d - |V_1|, |V_2|\}$. Since $1 \leq |V_2| \leq |V_1| < (\Delta - 1)^d$, we have $p \geq 1$. For $q = \lceil \frac{p}{\Delta - 1} \rceil$ let $y_1, y_2, \ldots, y_q$ (and $z_1, z_2, \ldots, z_q$, respectively) be the rightmost (leftmost) q vertices of T_{v_1} (T_{v_2}) on line $\mathbf{R} \times \{d - 1\}$ ($\mathbf{R} \times \{d\}$). Furthermore, let $x_1, x_2, \ldots, x_p$ be the p leftmost vertices in V_2. Let T' be the tree with vertex set $V(T)$ and edge set

$$E(T') = (E(T) \setminus \{x_j z_{\lceil j/(\Delta-1) \rceil} \mid 1 \leq j \leq p\}) \cup \{x_j y_{\lceil j/(\Delta-1) \rceil} \mid 1 \leq j \leq p\}.$$

Going from T to T' the sum of the distances between all pairs of vertices in $V(T) \setminus \{x_1, x_2, \ldots, x_p\}$ and between all pairs of vertices in $\{x_1, x_2, \ldots, x_p\}$ remain unchanged. This implies

$$\sigma(T) - \sigma(T') = \sum_{\substack{x \in \{x_1, x_2, \ldots, x_p\} \\ y \in V(T) \setminus \{x_1, x_2, \ldots, x_p\}}} (d_T(x, y) - d_{T'}(x, y)).$$

For $x \in \{x_1, x_2, \ldots, x_p\}$, $y \in V(T) \setminus (V(T_{v_1}) \cup V(T_{v_2}))$ and $y' \in V_3$ we have $d_T(x, y) - d_{T'}(x, y) = 1$ and $d_T(x, y') - d_{T'}(x, y') = -1$.
If $\{v\} \neq C(T)$, then $|V(T) \setminus (V(T_{v_1}) \cup V(T_{v_2}))| > |V(T) \setminus V(T_v)| \geq |V(T_v)| > |V_3|$ in view of the definition of the centroid and the tree T_v. If $\{v\} = C(T)$, then we obtain

$$|V(T) \setminus (V(T_{v_1}) \cup V(T_{v_2}))| \geq 1 + \sum_{i=0}^{d-1} (\Delta - 2)(\Delta - 1)^i \geq |V_3|.$$

Thus, in both cases we obtain

$$\sum_{\substack{x\in\{x_1,x_2,\dots,x_p\}\\ y\in V(T)\setminus(V(T_{v_1})\cup V(T_u))}} (d_T(x,y)-d_{T'}(x,y)) \;=\; p\cdot|V(T)\setminus(V(T_{v_1})\cup V(T_{v_2}))| \,-\, p\cdot|V_3|\geq 0.$$

Now, it remains to consider

$$\sum_{\substack{x\in\{x_1,x_2,\dots,x_p\}\\ y\in V(T_{v_1})\cup V(T_u)}} (d_T(x,y)-d_{T'}(x,y)).$$

The tree $T'[V(T_{v_1})\cup\{x_1,x_2,...,x_p\}]$ contains a tree $T_u^*\cong T_u$ as a subgraph such that $\{x_1,x_2,...,x_p\}\subseteq V(T_u^*)$. Let $V_1^*=V_1\setminus V(T_u^*)$. Note that $V_1^*\neq\emptyset$ and that $V_1^*=V_1$ if $p=|V_2|$. Thus,

$$\sum_{\substack{x\in\{x_1,x_2,\dots,x_p\}\\ y\in(V(T_{v_1})\cup V(T_u))\setminus V_1^*}} (d_T(x,y)-d_{T'}(x,y))=0$$

and

$$\sum_{\substack{x\in\{x_1,x_2,\dots,x_p\}\\ y\in V_1^*}} (d_T(x,y)-d_{T'}(x,y))\geq p\cdot|V_1^*|\cdot((2d+1)-(2d-2))>0.$$

Hence, we obtain

$$\begin{aligned}\sigma(T)-\sigma(T') \;&\geq\; \sum_{\substack{x\in\{x_1,x_2,\dots,x_p\}\\ y\in V(T_{v_1})\cup V(T_u)}} (d_T(x,y)-d_{T'}(x,y))\\ &=\; \sum_{\substack{x\in\{x_1,x_2,\dots,x_p\}\\ y\in V_1^*}} (d_T(x,y)-d_{T'}(x,y))>0.\end{aligned}$$

which is a contradiction to the choice of T. This completes the proof in this case.

Case 2. The distance of any two endvertices in T_v from v differs by at most one.

Let $M_k(R,\Delta)\leq|V(T_v)|<M_{k+1}(R,\Delta)$ for some $k\geq 1$. The above claim implies that the tree T arises from the tree T_0 in $\mathcal{T}(R,\Delta)$ of order $M_k(R,\Delta)$ by attaching $n-M_k(R,\Delta)$ endvertices that lie on the line $\mathbf{R}\times\{k+1\}$ to the vertices of T_0 that lie on the line $\mathbf{R}\times\{k\}$. By the Lemma 2.4, we obtain that desired result. This completes the proof in this case and the proof of the theorem is complete.
□

Now we come to the proof of Theorem 2.2.

Proof of Theorem 2.2: If $|C(T)|=1$, then Theorem 2.5 immediately implies Theorem 2.2. Now let $C(T)=\{c_1,c_2\}$. By Theorem 2.3, the trees T_{c_1} and T_{c_2} both have exactly $\frac{n}{2}$ vertices and by Theorem 2.5, $T_{c_1},T_{c_2}\in\mathcal{T}(\Delta-1,\Delta)$. This implies that T_{c_1} and T_{c_2} are isomorphic. It follows that $|V(T_{c_1})|=|V(T_{c_2})|=M_k(\Delta-1,\Delta)$ for some $k\geq 0$, otherwise

Lemma 2.4 would provide a tree, which is better than the optimal. This implies that $T \in \mathcal{T}(\Delta, \Delta)$ and the proof is complete.
$\square$

If $T \in \mathcal{T}(\Delta, \Delta)$ has order $n = M_k(\Delta, \Delta)$ for some $k \geq 1$, then a tedious but straightforward calculation yields

$$\begin{aligned} \bar{d}(T) &= \frac{2 \cdot [(\Delta-1)^{2k}(k\Delta(\Delta-2) - 2\Delta + 1) + (\Delta-1)^k 2\Delta - 1]}{(\Delta-2) \cdot [\Delta(\Delta-1)^{2k} - (\Delta+2)(\Delta-1)^k + 2]} \\ &= (1+o(1)) \cdot 2k \qquad (\Delta \to \infty) \\ &= (1+o(1)) \cdot \log_{\Delta-1} \frac{1}{\Delta}((\Delta-2)n+2) \qquad (\Delta \to \infty). \end{aligned}$$

At the end of this section we want to mention another extremal property of the trees in $\mathcal{T}(\Delta, \Delta)$. For a graph G let $\tilde{\sigma}(G) = \min\{\sigma_G(v) | v \in V(G)\}$. The straightforward proof is left to the reader.

Proposition 2.6 *Let T be a tree of order n and maximum degree $\Delta \geq 3$. If $\tilde{\sigma}(T) \leq \tilde{\sigma}(T')$ for all trees T' of order n and maximum degree Δ, then $T \in \mathcal{T}(\Delta, \Delta)$.*

3 Trees with maximum Wiener Index

A tree is a *caterpillar* if the deletion of its endvertices produces a path. A caterpillar of order n whose vertices are either endvertices or of degree Δ will be denoted by $C(n, \Delta)$ (note that $n \equiv 2 \bmod (\Delta - 1)$). Let $x(n, \Delta)$ denote an endvertex of $C(n, \Delta)$ such that the neighbour of $x(n, \Delta)$ has at most one neighbour of degree Δ. The following theorem settles Problem 1.2.

Theorem 3.1 *Let T be a tree of order n such that $d_T(x) \in \{1, \Delta\}$ for all $x \in V(T)$ and some $\Delta \geq 3$.*

a) Let $x \in V(T)$ be such that $\sigma_T(x) = \max\{\sigma_T(y) | y \in V(T)\}$. Then

$$\sigma_T(x) \leq \sigma_{C(n,\Delta)}(x(n, \Delta))$$

with equality if and only if there is an isomorphism between T and $C(n, \Delta)$ that maps x on $x(n, \Delta)$.

b) $\sigma(T) \leq \sigma(C(n, \Delta))$ with equality if and only if T and $C(n, \Delta)$ are isomorphic.

Proof: a) The proof of this part is straightforward and we leave it to the reader.

b) We assume that T maximizes the Wiener index among all trees of order n whose vertices are either endvertices or of maximum degree. Furthermore, we assume that T is a counterexample of minimum order, i.e. $T \not\cong C(n, \Delta)$ and the conclusion of the theorem holds for all orders $< n$.

This implies that there is a vertex $x \in V(T)$ of maximum degree such that for some $k \geq 3$ the vertices $y_1, y_2, ..., y_k$ are the neighbours of x of maximum degree. For $1 \leq i \leq k$ let V_i be the vertex set of the component of $T[V(T) \setminus \{x\}]$ that contains y_i and let $T_i = T[V_i \cup \{x\}]$.

We assume that for some $1 \leq i \leq k$ there is no isomorphism between T_i and $C(n(T_i), \Delta)$ that maps x on $x(n(T_i), \Delta)$. Let T' be a tree on the vertex set of T such that

$$T'[V(T) \setminus V_i] \cong T[V(T) \setminus V_i]$$

and there is an isomorphism between $T'_i = T'[V_i \cup \{x\}]$ and $C(n(T_i), \Delta)$ that maps x on $x(n(T_i), \Delta)$. We have

$$\sigma(T) = \sigma(T_i) + \sigma(T[V(T) \setminus V_i]) + |V_i| \cdot \sigma_{T[V(T) \setminus V_i]}(x) + |V(T) \setminus (V_i \cup \{x\})| \cdot \sigma_{T_i}(x)$$

and

$$\sigma(T') = \sigma(T'_i) + \sigma(T[V(T) \setminus V_i]) + |V_i| \cdot \sigma_{T[V(T) \setminus V_i]}(x) + |V(T) \setminus (V_i \cup \{x\})| \cdot \sigma_{T'_i}(x).$$

Therefore

$$\sigma(T) - \sigma(T') = \sigma(T_i) - \sigma(T'_i) + |V(T) \setminus (V_i \cup \{x\})| \cdot (\sigma_{T_i}(x) - \sigma_{T'_i}(x)).$$

If $T_i \not\cong C(n(T_i), \Delta)$, then $\sigma(T'_i) > \sigma(T_i)$, since T is a minimum counterexample. Furthermore, by part a), $\sigma_{T'_i}(x) > \sigma_{T_i}(x)$ and we have $\sigma(T') > \sigma(T)$ which is a contradiction. If $T_i \cong C(n(T_i), \Delta)$, then $\sigma(T'_i) = \sigma(T_i)$. Furthermore, by part a), $\sigma_{T'_i}(x) > \sigma_{T_i}(x)$ and we have $\sigma(T') > \sigma(T)$ which again is a contradiction.

Hence for all $1 \leq i \leq k$ there is an isomorphism between T_i and $C(n(T_i), \Delta)$ that maps x on $x(n(T_i), \Delta)$.

Now let z be an endvertex of T in V_2 such that the neighbour of z has at most one neighbour of maximum degree. Let the tree T' (see Figure 3 for an example of the construction) have vertex set $V(T)$ and edge set

$$E(T') = (E(T) \setminus \{ay_1 | a \in N_T(y_1) \setminus \{x\}\}) \cup \{az | a \in N_T(y_1) \setminus \{x\}\}.$$

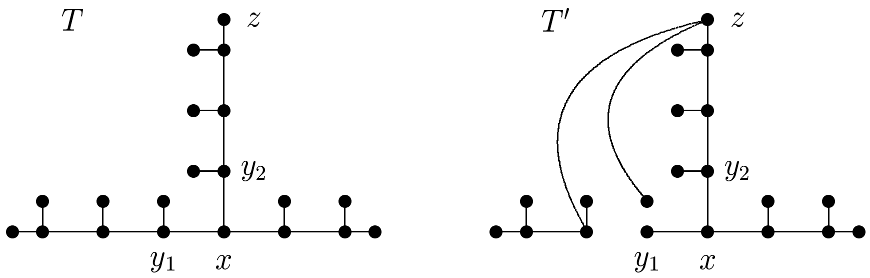

Figure 3

In view of the structure of the trees $C(n(T_i), \Delta)$ it is now trivial to see that again $\sigma(T') > \sigma(T)$ which is a contradiction and the proof is complete. □

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