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WIENER INDEX OF TREES OF GIVEN ORDER AND DIAMETER AT MOST 6

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Abstract

The long-standing open problem of finding an upper bound for the Wiener index of a graph in terms of its order and diameter is addressed. Sharp upper bounds are presented for the Wiener index, and the related degree distance and Gutman index, for trees of order n and diameter at most 6.

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1. Introduction

Let G be a graph with vertex set $V(G)$ and order n. We denote the distance between two vertices u, v in G by $d_G(u, v)$ (or simply $d(u, v)$); the diameter of G will be denoted by $d(G)$ (or d), the eccentricity of a vertex v will be denoted by $\mathrm{ec}(v)$ and the degree of v will be denoted by $\deg(v)$. Let $N_i^G(v)$ (or simply $N_i(v)$) be the set of vertices at distance i from v in G. Let u, v be two adjacent (nonadjacent) vertices of a graph G. Then $G' = G - uv$ ($G' = G + uv$) is obtained by removing the edge uv from G (by adding the edge uv to G).

The Wiener index is the oldest topological index. It has been investigated in the mathematical, chemical and computer science literature since the 1940s. The Wiener index $W(G)$ of a connected graph G is defined as the sum of the distances between all unordered pairs of vertices. The minimum value of the Wiener index of a graph (of a tree) of given order is attained by the complete graph (by the star), and the maximum value is attained by the path.

The degree distance, a variant of the Wiener index, is defined as

$$D'(G) = \sum_{\{u,v\}\subseteq V(G)} (\deg(u) + \deg(v))\, d(u, v),$$

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and the Gutman index is defined as

$$\mathrm{Gut}(G) = \sum_{\{u,v\}\subseteq V(G)} \deg(u)\deg(v)\, d(u, v).$$

The smallest value of the degree distance and Gutman index of graphs of order n is attained by stars (see [1, 11]). Turning to upper bounds on the degree distance, in 1999 Tomescu [11] conjectured the asymptotic upper bound $D'(G) \le (1/27)n^4 + O(n^3)$. Nine years later, Bucicovschi and Cioabă [2] commented that Tomescu's conjecture 'seems difficult at present time'. In the following year Dankelmann *et al.* [3] considered this problem and though they came close to proving the conjecture, their proof was inadequate to meet the $O(n^3)$ error term. Recently, Morgan *et al.*, in a submitted paper ('On a conjecture by Tomescu'), salvaged enough from the proof given in [3] and solved Tomescu's conjecture completely. There one can also find upper bounds on the degree distance of graphs of given order and diameter. Upper bounds on the Gutman index of a graph of given order and diameter were studied in [4, 9]. In [9] it was proved, that $\mathrm{Gut}(G) \le (1/16)d(n-d)^4 + O(n^4)$ and consequently $\mathrm{Gut}(G) \le (2^4/5^5)n^5 + O(n^4)$.

In this paper we study the indices mentioned above for trees of given order and diameter. Since Klein *et al.* [7] showed that for every tree T of order n,

$$D'(T) = 4W(T) - n(n-1), \tag{1.1}$$

and in [6] Gutman proved that

$$\mathrm{Gut}(T) = 4W(T) - (2n-1)(n-1), \tag{1.2}$$

any result on $W(T)$ yields a similar result on $D'(T)$ and $\mathrm{Gut}(T)$. It is not difficult to show that the extremal tree, which has the minimum Wiener index among trees of order n and diameter d, is the path of length d (containing $d + 1$ vertices) with the central vertex joined to the other $n - d - 1$ vertices; see [12].

The problem of finding an upper bound on the Wiener index of a tree (or graph) in terms of order and diameter is quite challenging; it was addressed by Plesník [10] in 1975, and restated by DeLaViña and Waller [5], but still remains unresolved to this date. In this paper, we give a starting point to solving this long-standing problem. We present upper bounds on the Wiener index of trees of order n and diameter at most 6, and we show that our bounds are best possible. As a corollary we obtain upper bounds on the degree distance and Gutman index of trees of given order and diameter at most 6. Let us mention that there are indices which were introduced much later than the Wiener index, however upper bounds on these indices for trees of given order and diameter are known. For example, a sharp upper bound on the eccentric connectivity index of trees of given order and diameter was given in [8]. To find a sharp upper bound on the Wiener index for trees of given order and large diameter seems to be a very complicated problem.

2. Preliminary results

First we give a few results which will be used in proofs of our main theorems. Note that

$$W(T)=\sum_{\{u,v\}\subseteq V(T)} d(u,v)=\frac{1}{2}\sum_{u\in V(T)}\sum_{v\in V(T)} d(u,v)=\frac{1}{2}\sum_{u\in V(T)}\sum_{i=1}^{d} i|N_i^T(u)|.$$

Lemma 2.1. *Let T be a tree of diameter $2r$ ($r\geq 2$) with the central vertex v, and let $\deg(u)=2$ for every vertex $u\in N_i(v)$ where $i=1,2,\ldots,r-2$. If T has the maximum Wiener index among trees of given order and diameter $2r$, then the degrees of any two vertices in $N_{r-1}(v)$ differ by at most one.*

Proof. Let u_1,u_2 be any two vertices in $N_{r-1}^T(v)$, and let n_i be the number of leaves adjacent to u_i in T, $i=1,2$. We prove the result by contradiction. Suppose that $n_1\geq n_2+2$. We show that T does not have the maximum Wiener index among trees of given order and diameter $2r$. Let w be any leaf adjacent to u_1 in T, and let $T'=T-u_1w+u_2w$. We have $V(T')=V(T)$, $d(T')=d(T)=2r$, $d_T(w_1,w_2)=d_{T'}(w_1,w_2)$ for any two vertices w_1,w_2 different from w, and $|N_i^T(w)|\neq|N_i^{T'}(w)|$ only if $i=2$ or $2r$. Since $|N_2^T(w)|=n_1$, $|N_2^{T'}(w)|=n_2+1$ and $|N_{2r}^{T'}(w)|-|N_{2r}^T(w)|=(n_1-1)-n_2$,

$$\begin{aligned}W(T')-W(T)&=2r(|N_{2r}^{T'}(w)|-|N_{2r}^T(w)|)+2(|N_2^{T'}(w)|-|N_2^T(w)|)\\&=2(r-1)(n_1-n_2-1)>0,\end{aligned}$$

which is a contradiction. □

Corollary 2.2. *Let T_1 be a join of a tree T (which is defined in the previous lemma) and any tree T_2, where T_1 is constructed in such a way that we unify the central vertex of T with any vertex of T_2. If T_1 has the maximum Wiener index among trees of given order and diameter, then the degrees of any two vertices in $N_{r-1}(v)$ which are in T differ by at most one.*

Lemma 2.3. *Let T be a tree of diameter $2r$ ($r\geq 2$) with the central vertex v, and let $\deg(u)=2$ for every vertex $u\in N_i(v)$ where $i=1,2,\ldots,r-2$. Let $|N(v)|=k$ and $|N_r(v)|=n_k$. If T has the maximum Wiener index among trees of given order and diameter $2r$, then*

$$\sum_{\{y,x\}\subseteq N_r(v)} d(y,x)\leq n_k\Big(rn_k+(1-r)\frac{n_k}{k}-1\Big),$$

and we have the equality only if the degrees of all vertices in $N_{r-1}(v)$ are equal.

Proof. Let T be a tree with $\deg(u)=2$ for every vertex $u\in N_i(v)$ where $i=1,2,\ldots,r-2$ and let $|N(v)|=k$. Then $|N_i(v)|=k$ for any $i=2,3,\ldots,r-1$. Let $N_{r-1}(v)=\{v_1,v_2,\ldots,v_k\}$. By Lemma 2.1, if T has the maximum Wiener index, then v_j ($j=1,2,\ldots,k$) has either $s-1$ or s neighbours in $N_r(v)$ for some $s\geq 1$. Without loss of generality, we can assume that the number of vertices in $N_r(v)$ which are adjacent to v_i ($i = 1, 2, \ldots, p$, $1 \le p \le k$) is $s-1$, and the number of vertices in $N_r(v)$ which are adjacent to v_j ($j = p+1, p+2, \ldots, k$) is s. We have $n_k = p(s-1) + (k-p)s = ks - p$. Then any two vertices in $N_r(v)$ are of distance 2 if they have a common neighbour in $N_{r-1}(v)$, otherwise they are of distance $2r$. Hence, for $w, w' \in N_r(v)$,

$$\sum_{x \in N_r(v)} d(w, x) = 2(s-2) + 2r(ks - p - s + 1) \quad \text{if } w \in N(v_i),\ i = 1, 2, \ldots, p,$$
$$\sum_{x \in N_r(v)} d(w', x) = 2(s-1) + 2r(ks - p - s) \quad \text{if } w' \in N(v_j),\ j = p+1, p+2, \ldots, k,$$

which yields

$$\begin{aligned} 2 \sum_{\{y,x\} \subseteq N_r(v)} d(y, x) &= \sum_{y \in N_r(v)} \sum_{x \in N_r(v)} d(y, x) \\ &= p(s-1) \sum_{x \in N_r(v)} d(w, x) + (k-p)s \sum_{x \in N_r(v)} d(w', x) \\ &= (ks - p)(2r(ks - p) + 2(1-r)s - 2) + 2p(s-1)(r-1). \end{aligned}$$

Since $p/k \le 1$, we have $s - 1 \le s - p/k$, and consequently

$$2p(s-1)(r-1) \le 2p\Big(s - \frac{p}{k}\Big)(r-1) = \frac{2p}{k}(ks - p)(r-1).$$

Hence

$$\begin{aligned} \sum_{\{y,x\} \subseteq N_r(v)} d(y, x) &\le \frac{ks - p}{2}\Big(2r(ks - p) + 2(1-r)s + \frac{2p}{k}(r-1) - 2\Big) \\ &= n_k\Big(rn_k + (1-r)\frac{n_k}{k} - 1\Big). \end{aligned}$$

Clearly we have equality above only if $p/k = 1$, which means that every vertex in $N_{r-1}(v)$ is adjacent to $s-1$ vertices in $N_r(v)$. □

Corollary 2.4. *Let T_1 be a join of a tree T (defined as in Lemma 2.3) and a new tree T_2, where T_1 is constructed in such a way that we unify the central vertex of T with any vertex of T_2. Then the distances between vertices in T do not change, and if T_1 has the maximum Wiener index among trees of given order and diameter, then*

$$\sum_{\{y,x\} \subseteq N_r^T(v)} d(y, x) \le n_k\Big(rn_k + (1-r)\frac{n_k}{k} - 1\Big),$$

and we have equality only if the degrees of all vertices in $N_{r-1}^T(v)$ are equal.

Lemma 2.5. *Let $u_1, u_2, \ldots, u_k$ be any set of vertices of a tree T which have a common neighbour, and let all the other neighbours of u_i be leaves, $i = 1, 2, \ldots, k$. If T has the maximum Wiener index among trees of order n and diameter $d \ge 5$, then:*

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(i) *if* $k \geq 2$ *and* $\mathrm{ec}(u_i) < d$, *then* $|N(u_i)| + |N(u_j)| > \sqrt{2n} - 1$ *for any* $i, j \in \{1, 2, \ldots, k\}$, $i \neq j$;
(ii) $|N(u_i)| < \sqrt{2n} + 1$ *for any* $i \in \{1, 2, \ldots, k\}$.

PROOF. Let u be a neighbour of all u_i, $i = 1, 2, \ldots, k$, and let $U_i = N(u_i) \setminus \{u\}$. We prove by contradiction that $|U_i| < \sqrt{2n}$ and if $k \geq 2$ and $\mathrm{ec}(u_i) < d$, then $|U_i| + |U_j| > \sqrt{2n} - 3$ for any $i, j \in \{1, 2, \ldots, k\}$, $i \neq j$.

(i) Suppose that there are 2 vertices u_i, u_j such that $|U_i| + |U_j| \leq \sqrt{2n} - 3$. Let

$$T' = T - \bigcup_{w \in U_j} u_j w - u u_j + \bigcup_{w \in U_j} u_i w + u_i u_j.$$

Note that if we do not assume that $\mathrm{ec}(u_i) < d(T)$, then u_i can be the end vertex of a diametral path in T, which implies $d(T) < d(T')$. We also know that (since $d(T) \geq 5$) there is a vertex, say y, such that $d_T(v, y) = d_{T'}(v, y) \geq 3$, and hence $d(T')$ cannot be less than 5. It follows that $d(T) = d(T')$ and $d_T(w_1, w_2) = d_{T'}(w_1, w_2)$ for any two vertices w_1, w_2 except for the cases when $w_1 \in U_i \cup \{u_i\}$ and $w_2 \in U_j$, or when $w_1 = u_j$. We have

$$\begin{aligned} d_{T'}(w_1, w_2) &= d_T(w_1, w_2) - 2 \quad \text{if } w_1 \in U_i \cup \{u_i\}, w_2 \in U_j, \\ d_{T'}(u_j, w) &= d_T(u_j, w) - 1 \quad \text{if } w \in U_i \cup \{u_i\}, \\ d_{T'}(u_j, w) &= d_T(u_j, w) + 1 \quad \text{if } w \in V(T) \setminus (U_i \cup \{u_i, u_j\}). \end{aligned}$$

Hence

$$\begin{aligned} W(T') - W(T) &= \sum_{w_1 \in U_i \cup \{u_i\}} \sum_{w_2 \in U_j} (d_{T'}(w_1, w_2) - d_T(w_1, w_2)) \\ &\quad + \sum_{w \in V(T)} (d_{T'}(u_j, w) - d_T(u_j, w)) \\ &= -2(|U_i| + 1)|U_j| - (|U_i| + 1) + (n - |U_i| - 2) \\ &= n - 2|U_i||U_j| - 2|U_i| - 2|U_j| - 3. \end{aligned} \tag{2.1}$$

Since $|U_i||U_j| \leq ((|U_i| + |U_j|)/2)^2$,

$$W(T') - W(T) \geq n - 2\Big(\frac{\sqrt{2n} - 3}{2}\Big)^2 - 2(\sqrt{2n} - 3) - 3 = \sqrt{2n} - \frac{3}{2} > 0.$$

Hence T is not a graph with the maximum Wiener index.

(ii) Suppose that $|U_i| \geq \sqrt{2n}$ for some $i \in \{1, 2, \ldots, k\}$. Let $x \in U_i$, and let X and Y be two disjoint subsets of U_i such that $|X|$ and $|Y|$ differ by at most 1, and $U_i = X \cup Y \cup \{x\}$. Then $|X|, |Y| \geq \sqrt{n/2} - 1$. Let

$$T' = T - \bigcup_{w \in X} u_i w - u_i x + u x + \bigcup_{w \in X} x w.$$

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Then $d_T(w_1, w_2) \neq d_{T'}(w_1, w_2)$ only in the following cases:

$$\begin{aligned} d_{T'}(w_1, w_2) &= d_T(w_1, w_2) + 2 \quad \text{if } w_1 \in Y \cup \{u_i\}, w_2 \in X, \\ d_{T'}(x, w) &= d_T(x, w) + 1 \quad \text{if } w \in Y \cup \{u_i\}, \\ d_{T'}(x, w) &= d_T(x, w) - 1 \quad \text{if } w \in V(T) \setminus (Y \cup \{u_i, x\}). \end{aligned}$$

Hence

$$\begin{aligned} W(T) - W(T') &= \sum_{w_1 \in Y \cup \{u_i\}} \sum_{w_2 \in X} (d_T(w_1, w_2) - d_{T'}(w_1, w_2)) + \sum_{w \in V(T)} (d_T(x, w) - d_{T'}(x, w)) \\ &= -2(|Y| + 1)|X| - (|Y| + 1) + (n - |Y| - 2) \\ &= n - 2|X||Y| - 2|X| - 2|Y| - 3 \\ &= n - 2|X||Y| - 2|U_i| - 1 \\ &\leq n - 2\Big(\sqrt{\frac{n}{2}} - 1\Big)^2 - 2\sqrt{2n} - 1 = -3, \end{aligned}$$

which is a contradiction. □

3. Main results

We present results on the Wiener index of trees of given order and diameter at most 6. The only tree of order n and diameter 2 is the star S_n having $n - 1$ leaves. Since any two leaves of the star are at distance 2, and the distance between the central vertex and any leaf is 1, the Wiener index of S_n is $2\binom{n-1}{2} + (n - 1) = n^2 - 2n + 1$. Then from (1.1) and (1.2) it follows that the degree distance of the star is $D'(S_n) = 3n^2 - 7n + 4$ and the Gutman index is $\mathrm{Gut}(S_n) = 2n^2 - 5n + 3$.

Now we bound the Wiener index for diameter d where $3 \leq d \leq 6$.

Theorem 3.1. *Let T be a tree of order n and diameter* 3. *Then the Wiener index of T is*

$$W(T) \leq \frac{5n^2}{4} - 3n + 3$$

and this bound is best possible.

Proof. Let T be any tree of order n and diameter 3. We denote the central vertices of T by v and u. The set of leaves adjacent to v (to u) will be denoted by K (by L). Let $|K| = k$. Then $|L| = n - k - 2$. It can be checked that

$$\sum_{\{y,x\} \subseteq K} d(y, x) = 2\binom{k}{2}, \quad \sum_{\{y,x\} \subseteq L} d(y, x) = 2\binom{n-k-2}{2}, \quad \sum_{y \in K} \sum_{x \in L} d(y, x) = 3k(n - k - 2),$$
$$\sum_{x \in V(T)} d(v, x) = (k + 1) + 2(n - k - 2) \quad \text{and} \quad \sum_{x \in V(T)} d(u, x) = (n - k - 1) + 2k,$$

which yield

$$W(T) = \sum_{\{y,x\}\subseteq K} d(y,x) + \sum_{\{y,x\}\subseteq L} d(y,x) + \sum_{y\in K}\sum_{x\in L} d(y,x) + \sum_{x\in V(T)} d(v,x) + \sum_{x\in V(T)} d(u,x)$$
$$= n^2 - 2n + kn - k^2 - 2k + 2 = f(k).$$

Then from the derivative $f'(k) = 0$ we obtain $k = n/2 - 1$, which yields the maximum of $f(k)$. Hence

$$W(T) \le f\Big(\frac{n}{2} - 1\Big) = \frac{5n^2}{4} - 3n + 3.$$

This value is attained by the Wiener index of a tree which has both central vertices of degree $n/2$. Therefore our bound is best possible. □

THEOREM 3.2. *Let T be a tree of order n and diameter 4. Then*

$$W(T) \le 2n^2 - 2n\sqrt{n-1} - 3n + 2\sqrt{n-1} + 1$$

and the bound is best possible.

PROOF. Let T be a tree with the maximal Wiener index among all trees of order n and diameter 4. We denote the central vertex of T by v. Let $|N(v)| = k$ and $|N_2(v)| = n_k$. Clearly $|V(T)| = n = 1 + k + n_k$. By Lemma 2.3,

$$\sum_{\{y,x\}\subseteq N_2(v)} d(y,x) \le n_k\Big(2n_k - \frac{n_k}{k} - 1\Big). \tag{3.1}$$

It is easy to check that

$$\sum_{\{y,x\}\subseteq N(v)} d(y,x) = 2\binom{k}{2}, \qquad \sum_{y\in N_2(v)}\sum_{x\in N(v)} d(y,x) = n_k(1 + 3(k-1))$$

and

$$\sum_{x\in V(T)} d(v,x) = k + 2n_k.$$

Consequently,

$$W(T) = \sum_{\{y,x\}\subseteq N_2(v)} d(y,x) + \sum_{\{y,x\}\subseteq N(v)} d(y,x) + \sum_{y\in N_2(v)}\sum_{x\in N(v)} d(y,x) + \sum_{x\in V(T)} d(v,x)$$
$$\le 2n_k^2 - \frac{n_k^2}{k} + (3k-1)n_k + k^2$$
$$= 2n^2 - \frac{(n-1)^2}{k} - kn - 3n + k + 1 = f(k).$$

Then the derivative $f'(k) = 0$ yields the value $k = \sqrt{n-1}$, which gives us the maximum of $f(k)$. It follows that

$$W(T) \le 2n^2 - 2n\sqrt{n-1} - 3n + 2\sqrt{n-1} + 1. \tag{3.2}$$

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Note that our bound is best possible. If every vertex in $N[v]$ is of degree $\sqrt{n-1}$, where $n-1$ is a square, then by Lemma 2.3 we have equality in (3.1), and consequently equality in (3.2) as well. □

THEOREM 3.3. *Let T be a tree of order n and diameter 5. Then the Wiener index*

$$W(T) \le \frac{9n^2}{4} - 2n^{3/2} + O(n)$$

and the bound is best possible.

PROOF. Let T be a tree with the maximal Wiener index among all trees of order n and diameter 5. We denote the central vertices of T by v and u. Let $K_1 = N(v) \setminus \{u\}$, $L_1 = N(u) \setminus \{v\}$, and let K_2 (L_2) contain every leaf which has a neighbour in K_1 (in L_1). Clearly $V(T) = \{v, u\} \cup K_1 \cup L_1 \cup K_2 \cup L_2$. Let $|K_1| = k$, $|L_1| = l$, $|K_3| = n_k$ and $|L_3| = n_l$.

Claim 1. We show that

$$W(T) \le 2(n_k + n_l)^2 + n_k n_l - \frac{n_k^2}{k} - \frac{n_l^2}{l} + 3(k+l)(n_k + n_l) \\ + l n_k + k n_l + k^2 + l^2 + 3kl + 2k + 2l + 1.$$

From Corollary 2.4 it follows that

$$\sum_{\{x,y\} \subseteq K_2} d(x,y) \le n_k\Big(2n_k - \frac{n_k}{k} - 1\Big) \quad \text{and} \quad \sum_{\{x,y\} \subseteq L_2} d(x,y) \le n_l\Big(2n_l - \frac{n_l}{l} - 1\Big).$$

It can be checked that

$$\sum_{x \in K_2} \sum_{y \in K_1 \cup L_1 \cup \{v,u\}} d(x,y) = n_k(1 + 2 + 3k + 4l),$$
$$\sum_{x \in L_2} \sum_{y \in K_1 \cup L_1 \cup \{v,u\}} d(x,y) = n_l(1 + 2 + 3l + 4k),$$
$$\sum_{x \in K_2} \sum_{y \in L_2} d(x,y) = 5 n_k n_l, \qquad \sum_{x \in K_1} \sum_{y \in L_1} d(x,y) = 3kl,$$
$$\sum_{\{x,y\} \subseteq K_1} d(x,y) = 2\binom{k}{2} = k(k-1), \qquad \sum_{\{x,y\} \subseteq L_1} d(x,y) = 2\binom{l}{2} = l(l-1),$$
$$\sum_{x \in K_1 \cup L_1} d(v,x) = k + 2l, \quad \sum_{x \in K_1 \cup L_1} d(u,x) = l + 2k \quad \text{and} \quad d(u,v) = 1.$$

Hence

$$W(T) \le 2(n_k + n_l)^2 + n_k n_l - \frac{n_k^2}{k} - \frac{n_l^2}{l} + 3(k+l)(n_k + n_l) \\ + l n_k + k n_l + k^2 + l^2 + 3kl + 2k + 2l + 1.$$

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By Lemma 2.5(i), if $k \geq 2$ (if $l \geq 2$), then $|N(x)| + |N(y)| > \sqrt{2n} - 1$ for any two vertices x, y in K_1 (in L_1). Since by Corollary 2.2 $|N(x)|$ and $|N(y)|$ differ by at most 1, both $|N(x)|$ and $|N(y)|$ are greater than $\sqrt{n/2 - 1}$. By Lemma 2.5(ii), $|N(x)|, |N(y)| < \sqrt{2n} + 1$. Hence if $k \geq 2$ (if $l \geq 2$) then we can assume that every vertex in K_1 (in L_1) is adjacent to $c_1\sqrt{n} + O(1)$ vertices in K_2, where $\sqrt{2}/2 \leq c_1 \leq \sqrt{2}$ (to $c_2\sqrt{n} + O(1)$ vertices in L_2, $\sqrt{2}/2 \leq c_2 \leq \sqrt{2}$). It follows that $n_k = k(c_1\sqrt{n} + O(1))$ and $n_l = l(c_2\sqrt{n} + O(1))$, and consequently $k \leq \sqrt{n}/c_1 + O(1)$ and $l \leq \sqrt{n}/c_2 + O(1)$ (since n_k and n_l cannot exceed n).

Claim 2. We have $n_k = n_l + O(n^{1/2})$.

Suppose to the contrary that $n_k > n_l + O(n^{1/2})$. Let w be any vertex in K_2, let v_1 be the neighbour of w in T ($v_1 \in K_1$), and let u_1 be any vertex in L_1. Let $T' = T - v_1w + u_1w$. We have $d(T') = d(T) = 5$,

$$\sum_{w' \in V(T)} d(w, w') = 1 + 2(c_1\sqrt{n} + O(1)) + 3k + 4(n_k - c_1\sqrt{n} - O(1)) + 4l + 5n_l$$
$$= 4n_k + 5n_l + O(n^{1/2})$$

and

$$\sum_{w' \in V(T')} d(w, w') = 4n_l + 5n_k + O(n^{1/2}).$$

Then

$$0 \leq W(T) - W(T') = \sum_{w' \in V(T)} d(w, w') - \sum_{w' \in V(T')} d(w, w') = n_l - n_k + O(n^{1/2}),$$

which is a contradiction.

Analogously it can be shown that n_l cannot be greater than $n_k + O(n^{1/2})$.

Since $n = n_k + n_l + k + l + 2 = n_k + n_l + O(n^{1/2})$, we have $n_k = n_l = n/2 + O(n^{1/2})$. We can write $n_k = n/2 + c_1'\sqrt{n} + O(1)$ and $n_l = n/2 + c_2'\sqrt{n} + O(1)$, where c_1' and c_2' are real numbers.

We also know that $n_k = k(c_1\sqrt{n} + O(1))$ which implies that $k = \sqrt{n}/2c_1 + O(1)$. Similarly we obtain $l = \sqrt{n}/2c_2 + O(1)$.

By Claim 1,

$$W(T) \leq 2(n_k + n_l)^2 + n_kn_l - \frac{n_k^2}{k} - \frac{n_l^2}{l} + 3(k + l)(n_k + n_l) + ln_k + kn_l + O(n),$$

and from the previous part of the proof it follows that

$$(n_k + n_l)^2 = (n - k - l - 2)^2 = n^2 - 2kn - 2ln + O(n),$$
$$\frac{n_k^2}{k} = \left(\frac{n}{2} + c_1'\sqrt{n} + O(1)\right)^2 \Big/ k = \frac{n^2}{4k} + O(n), \qquad \frac{n_l^2}{l} = \frac{n^2}{4l} + O(n),$$
$$(k + l)(n_k + n_l) = (k + l)n + O(n), \qquad kn_l + ln_k = (k + l)\frac{n}{2} + O(n).$$

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Since

$$n = n_k + n_l + k + l + 2 = \left(\frac{n}{2} + c_1'\sqrt{n}\right) + \left(\frac{n}{2} + c_2'\sqrt{n}\right) + k + l + O(1),$$

we obtain $(c_1' + c_2')\sqrt{n} = -k - l + O(1)$. Consequently,

$$n_k n_l = \frac{n^2}{4} + (c_1' + c_2')\sqrt{n}\,\frac{n}{2} + O(n) = \frac{n^2}{4} - (k + l)\frac{n}{2} + O(n).$$

It follows that

$$W(T) \le \frac{9n^2}{4} - (k + l)n - \frac{n^2}{4}\left(\frac{1}{k} + \frac{1}{l}\right) + O(n) = f(k, l).$$

Then the partial derivatives $f_k(k, l) = 0$ and $f_l(k, l) = 0$ show that $f(k, l)$ is maximised for $k = l = \sqrt{n}/2$. Hence

$$W(T) \le \frac{9n^2}{4} - 2n^{3/2} + O(n).$$

It can be checked that if $|K_1| = |L_1| = \sqrt{n-2}/2$ and every vertex in K_1 and L_1 is adjacent to $\sqrt{n-2} - 1$ leaves, where $n - 2$ is a power of 4, then $W(T) = 9n^2/4 - 2n^{3/2} + O(n)$. The proof is complete. □

Theorem 3.4. *Let T be a tree of order n and diameter 6. Then*

$$W(T) \le 3n^2 - 2\sqrt{6}n^{3/2} - 2n + O(n^{1/2})$$

and the bound is best possible.

Proof. Let T be a tree with the maximal Wiener index among all trees of order n and diameter 6. We denote the central vertex of T by v.

Note that instead of Claims 1 and 2 one could prove a more general claim saying that all leaves of T must be at distance 3 from v. However, we do not need such a result to prove our theorem.

Claim 1. There is no leaf joined to v.

Suppose to the contrary that x is a leaf joined to v. Since v is the central vertex of a tree of diameter 6, there must be at least two other vertices u_1, u_2 adjacent to v in T. Let U_i be the set which contains all vertices u that satisfy the inequality $d_T(u, u_i) < d_T(u, v)$, $i = 1, 2$. Then $U_1 \cap U_2 = \emptyset$. Since $|U_1| + |U_2| \le n - 2$, at least one set U_i contains at most $n/2 - 1$ vertices. Without loss of generality, we can suppose that $|U_1| \le n/2 - 1$. Let $T' = T - vx + u_1x$. Then $d(T') = d(T) = 6$ and

$$W(T') - W(T) = \sum_{u \in V(T)} (d_{T'}(x, u) - d_T(x, u)).$$

Since $d_{T'}(x, u) = d_T(x, u) - 1$ for any $u \in U_1$, and $d_{T'}(x, u') = d_T(x, u') + 1$ for any $u' \in V(T) \setminus (U_1 \cup \{x\})$, we get $W(T') > W(T)$.

Claim 2. The vertex v does not have a neighbour of degree two which is adjacent to a leaf.

Suppose that v has a neighbour x_1 of degree two which is adjacent to a leaf, say x_2. As in the previous claim, one can show that there must be a neighbour of v, say u_1, such that $d_T(u_1, u) < d_T(v, u)$ for at most $(n-3)/2$ vertices u of T. Then for $T' = T - vx_1 + u_1x_1$ we get $d_{T'}(x_i, u) = d_T(x_1, u) - 1$ for at most $(n-3)/2$ vertices u, and $d_{T'}(x_i, u') = d_T(x_i, u') + 1$ for at least $(n-1)/2$ vertices u' $(i = 1, 2)$. Consequently,

$$W(T') - W(T) = 2 \sum_{u \in V(T)} (d_{T'}(x_1, u) - d_T(x_1, u)) \geq 2.$$

Claim 3. Each neighbour of v has degree at most three.

Suppose to the contrary that v_1 is a neighbour of v, which is adjacent to at least three other vertices v_2, v_2' and v_2''. Let V_3 (V_3', V_3'') be the set of leaves adjacent to v_2 (v_2', v_2''). Without loss of generality, we can assume that $|V_3| \geq |V_3''| \geq |V_3'| \geq 0$. Let

$$T' = T - \bigcup_{w \in V_3'} wv_2' - v_1v_2' + \bigcup_{w \in V_3'} v_2w + v_2v_2'.$$

Analogous steps as the ones in the proof of Lemma 2.5(i) yield

$$W(T') - W(T) = n - 2|V_3||V_3'| - 2|V_3'| - 2|V_3'| - 3,$$

(see (2.1)). Note that if $|V_3| = |V_3'| = 0$, then $W(T') - W(T) > 0$, so we can assume that there is a vertex, say $v_3 \in V_3$.

Let $T'' = T - v_1v_2 + vv_3$. Then $d_T(w_1, w_2) \neq d_{T''}(w_1, w_2)$ in the following cases:

$$\begin{aligned} d_{T''}(w_1, w_2) &= d_T(w_1, w_2) + 2 \quad \text{if } w_1 \in V_3 \cup \{v_2\} \setminus \{v_3\}, w_2 \in V_3' \cup V_3'' \cup \{v_1, v_2', v_2''\} \\ d_{T''}(v_3, w) &= d_T(v_3, w) - 2 \quad \text{if } w \in V(T) \setminus (V_3 \cup V_3' \cup V_3'' \cup \{v_1, v_2, v_2', v_2''\}). \end{aligned}$$

Consequently,

$$\begin{aligned} W(T) - W(T'') &= -2|V_3|(|V_3'| + |V_3''| + 3) + 2(n - |V_3| - |V_3'| - |V_3''| - 4) \\ &= 2(n - |V_3||V_3'| - |V_3||V_3''| - 4|V_3| - |V_3'| - |V_3''| - 4). \end{aligned}$$

Since T has the maximum Wiener index among all graphs of order n and diameter d, we have $W(T') - W(T) \leq 0 \leq (W(T) - W(T''))/2$ which yields

$$\begin{aligned} 0 &\leq |V_3||V_3'| - |V_3||V_3''| - 2|V_3| + |V_3'| - |V_3''| - 1 \\ &= (|V_3| + 1)(|V_3'| - |V_3''|) - 2|V_3| - 1. \end{aligned}$$

Since $|V_3'| \leq |V_3''|$ and $|V_3| \geq 1$, we get a contradiction.

Let K_1 (L_1) be the set of neighbours of v which are of degree two (of degree three), and let K_i (L_i) be the set of vertices at distance i from v, such that every vertex in K_i (in L_i) has a neighbour in K_{i-1} (in L_{i-1}), $i = 2, 3$. Let $|K_1| = k$, $|L_1| = l$, $|K_3| = n_k$ and $|L_3| = n_l$. Clearly $n = 1 + 2k + 3l + n_k + n_l$.

Claim 4. For any two vertices v_2 and v_2' in K_2, where V_3 (V_3') is the set of neighbours of v_2 (of v_2') in K_3, we have $|V_3| + |V_3'| > \sqrt{3n} - 5$.

Let v_1 (v_1') be the vertex in K_1 adjacent to v_2 (to v_2'), and let V_3 (V_3') be the set of leaves adjacent to v_2 (to v_2'). Let

$$T' = T - \bigcup_{w \in V_3'} wv_2' - vv_1' - v_1'v_2' + \bigcup_{w \in V_3'} v_2w + v_2v_1' + v_2v_2'.$$

We mention all cases when $d_T(w_1, w_2) \neq d_{T''}(w_1, w_2)$. We have

$$\begin{aligned}
d_{T'}(w_1, w_2) &= d_T(w_1, w_2) - 4 \quad \text{if } w_1 \in V_3 \cup \{v_2\}, w_2 \in V_3',\\
d_{T'}(v_2', w) &= d_T(v_2', w) - 3 \quad \text{if } w \in V_3 \cup \{v_2\},\\
d_{T'}(v_1', w) &= d_T(v_1', w) - 2 \quad \text{if } w \in V_3 \cup \{v_2\},\\
d_{T'}(v_1, w) &= d_T(v_1, w) - 2 \quad \text{if } w \in V_3',\\
d_{T'}(v_1, v_2') &= d_T(v_1, v_2') - 1,\\
d_{T'}(v_2', w) &= d_T(v_2', w) + 1 \quad \text{if } w \in V(G) \setminus (V_3 \cup \{v_1, v_2, v_2'\})\\
d_{T'}(v_1', w) &= d_T(v_1', w) + 2 \quad \text{if } w \in V(G) \setminus (V_3 \cup V_3' \cup \{v_1, v_1', v_2, v_2'\}).
\end{aligned}$$

Then

$$\begin{aligned}
W(T') - W(T) &= 2(n - |V_3| - |V_3'| - 4) + (n - |V_3| - 3)\\
&\qquad - 1 - 2(|V_3| + |V_3'| + 1) - 3(|V_3| + 1) - 4(|V_3| + 1)|V_3'|\\
&= 3n - 4|V_3||V_3'| - 8|V_3| - 8|V_3'| - 17\\
&= 3n - 4\Big(\frac{|V_3| + |V_3'|}{2}\Big)^2 - 8(|V_3| + |V_3'|) - 17.
\end{aligned}$$

If $|V_3| + |V_3'| \leq \sqrt{3n} - 5$, then we get $W(T') - W(T) \geq 2(\sqrt{3n} - 1) > 0$. It can be checked that $d(T') \leq d(T)$. If $d(T') < d(T)$, it is easy to transform T' to T'' such that $V(T'') = V(T)$, $d(T'') = d(T)$ and $W(T'') > W(T') > W(T)$. So $W(T)$ is not the maximum Wiener index of trees of order n and diameter 6.

Claim 5. We have $l < \sqrt{n/2}$ and $k < \sqrt{3n}$.

By Claim 4, for the sets of neighbours V_3 and V_3' of any two vertices v_2 and v_2' in K_2 we have $|V_3| + |V_3'| > \sqrt{3n} - 5$. If k is even, then $n_k > (k/2)(\sqrt{3n} - 5)$. From Corollary 2.2 we know that $|V_3|$ and $|V_3'|$ differ by at most 1, so the number of leaves joined to any vertex in K_2 is greater than $\sqrt{3n}/2 - 3$. Hence, if k is odd,

$$n_k > \frac{k-1}{2}(\sqrt{3n} - 5) + \frac{\sqrt{3n}}{2} - 3 = \frac{k}{2}(\sqrt{3n} - 5) - \frac{1}{2}.$$

Then $n > 1 + 2k + (k/2)(\sqrt{3n} - 5) - 1/2$ which implies that $k < (2n - 1)/(\sqrt{3n} - 1) < (2 + \epsilon)n/\sqrt{3n}$ for some small $\epsilon > 0$. For us it suffices to use $\epsilon = 1$.

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By Lemma 2.5(i), if v_2 and v_2' are any two vertices in L_2 which have a common neighbour, where V_3 (V_3') is the set of neighbours of v_2 (of v_2') in L_3, then $|V_3| + |V_3'| > \sqrt{2n} - 3$. We get $n_l > (\sqrt{2n} - 3)l$ which yields $n > 1 + 3l + (\sqrt{2n} - 3)l$, and consequently $l < \sqrt{n/2}$.

Claim 6. Let $v_1, u_1 \in L_1$ and let V_3 (U_3) be a subset of L_3 containing vertices which are at distance 2 from v_1 (u_1). Then $|V_3|$ and $|U_3|$ differ by at most 1.

Suppose that $|V_3| \geq |U_3| + 2$. Let v_2', v_2'' (u_2', u_2'') be two vertices in L_2 adjacent to v_1 (u_1), and let V_3' (V_3'', U_3', U_3'') be the set of neighbours of v_2' (v_2'', u_2', u_2'') in L_3. Since $|V_3'| + |V_3''| \geq |U_3'| + |U_3''| + 2$, without loss of generality we can assume that $|V_3'| \geq |U_3'| + 1$. Let w be any vertex in V_3' and let $T' = T - v_2'w + u_2'w$. Since $|N_2^T(v_1) \cap L_3| \geq 2$, we have $|N_2^{T'}(v_1) \cap L_3| \geq 1$, which implies that there must be two vertices at distance 6 in T'. Hence $d(T) = d(T')$. It can be checked that $d_T(w_1, w_2) = d_{T'}(w_1, w_2)$ for any two vertices w_1, w_2 different from w, and $|N_i^T(w)| = |N_i^{T'}(w)|$ if $i = 1, 3, 5$. We have

$$\begin{aligned}
|N_2^{T'}(w)| - |N_2^T(w)| &= (|U_3'| + 1) - |V_3'|,\\
|N_4^{T'}(w)| - |N_4^T(w)| &= (|U_3''| + 1) - (|V_3''| + 1),\\
|N_6^{T'}(w)| - |N_6^T(w)| &= (|V_3| - 1) - |U_3|.
\end{aligned}$$

Then

$$\begin{aligned}
W(T') - W(T) &= \sum_{i=1}^{6} i(|N_i^{T'}(w)| - |N_i^T(w)|)\\
&= 6(|V_3| - |U_3|) - 4(|V_3''| - |U_3''|) - 2(|V_3'| - |U_3'|) - 4\\
&= 2(|V_3| - |U_3| - 2) + 2(|V_3'| - |U_3'|) \geq 2(|V_3'| - |U_3'|) > 0,
\end{aligned}$$

which is a contradiction.

Claim 7. We have

$$\sum_{\{x,y\}\subseteq L_3} d(x, y) \leq n_l\Big(3n_l - \frac{3n_l}{2l} - 1\Big).$$

Let $L_1 = \{v_1, v_2, \ldots, v_l\}$ and let v, u_i, w_i be the neighbours of v_i, $i = 1, 2, \ldots, l$. By Claim 6, the number of vertices in L_3 which are at distance 2 from v_i is either $2s$ or $2s + \epsilon$, where s is an integer, and $\epsilon = 1$ or -1. Without loss of generality, we can assume that the number of vertices in L_3 which are at distance 2 from v_j ($j = 1, 2, \ldots, p$, $0 \leq p \leq l$) is $2s + \epsilon$, and the number of vertices in L_3 which are at distance 2 from v_j ($j = p + 1, p + 2, \ldots, l$) is $2s$. Then by Corollary 2.2 we can assume that u_i ($i = 1, 2, \ldots, l$) and w_j ($j = p + 1, p + 2, \ldots, l$) are adjacent to s vertices in L_3, and w_j ($j = 1, 2, \ldots, p$) are adjacent to $s + \epsilon$ vertices in L_3. It follows that

$$|L_3| = n_l = (2l - p)s + p(s + \epsilon) = 2ls + \epsilon p.$$

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Then, for the vertices w, w', w'' in L_3,

$$\sum_{v'\in L_3} d(w, v') = 2(s-1) + 4s + 6(2ls + \epsilon p - 2s)$$
$$\text{if } w \in N(u_j) \cup N(w_j),\ j = p+1, p+2, \ldots, l,$$
$$\sum_{v'\in L_3} d(w', v') = 2(s-1) + 4(s+\epsilon) + 6(2ls + \epsilon p - 2s - \epsilon)$$
$$\text{if } w' \in N(u_i),\ i = 1, 2, \ldots, p,$$
$$\sum_{v'\in L_3} d(w'', v') = 2(s+\epsilon-1) + 4s + 6(2ls + \epsilon p - 2s - \epsilon)$$
$$\text{if } w'' \in N(w_i),\ i = 1, 2, \ldots, p,$$

which yield

$$\begin{aligned} 2\sum_{\{v'',v'\}\subseteq L_3} d(v'', v') &= \sum_{v''\in L_3}\sum_{v'\in L_3} d(v'', v') \\ &= 2(l-p)s\sum_{v'\in L_3} d(w, v') + ps\sum_{v'\in L_3} d(w', v') \\ &\quad + p(s+\epsilon)\sum_{v'\in L_3} d(w'', v') \\ &= (2ls + \epsilon p)(6(2ls+\epsilon p) - 6s - 2) - p(6\epsilon s + 4). \end{aligned}$$

Since $p/l \le 1$, we have $-p(6\epsilon s + 4) \le -p(6\epsilon s + 3p/l) = -(3\epsilon p/l)(2ls + \epsilon p)$. Consequently,

$$\sum_{\{w,u\}\subseteq L_3} d(w, u) \le \frac{2ls+\epsilon p}{2}\Big(6(2ls+\epsilon p) - 6s - \frac{3\epsilon p}{l} - 2\Big) = \frac{n_l}{2}\Big(6n_l - \frac{3n_l}{l} - 2\Big).$$

Claim 8. We have

$$\begin{aligned} W(T) \le{}& 3(n_k+n_l)^2 + (9k+14l)(n_k+n_l) - \frac{2n_k^2}{k} - \frac{3n_l^2}{2l} \\ &- 4n_k - 6n_l + 6k^2 + 15l^2 + 19kl - 2k - 6l. \end{aligned}$$

It can be checked that

$$\sum_{u\in K_3}\sum_{w\in L_3} d(u, w) = 6n_k n_l,$$
$$\begin{aligned} \sum_{u\in K_3}\sum_{w\in V(G)\setminus(K_3\cup L_3)} d(u, w) &= n_k(1+2+3+4(k-1)+4l+5(k-1)+5\cdot 2l) \\ &= n_k(9k+14l-3), \end{aligned}$$

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$$\sum_{u\in L_3}\sum_{w\in V(G)\setminus(K_3\cup L_3)} d(u,w) = n_l(1+2+3\cdot 2+4k+4(l-1)+5k+5\cdot 2(l-1))$$
$$= n_l(9k+14l-5),$$
$$\sum_{\{u,w\}\subseteq K_2} d(u,w) = 4\binom{k}{2} = 2k(k-1),$$
$$\sum_{\{u,w\}\subseteq L_2} d(u,w) = l(8l-6) \text{ since for any } u\in L_2,$$
$$\sum_{w\in L_2} d(u,w) = 2+4\cdot 2(l-1),$$
$$\sum_{u\in K_2}\sum_{w\in K_1\cup L_1\cup L_2\cup\{v\}} d(u,w) = k(1+2+3(k-1)+3l+4\cdot 2l) = k(3k+11l),$$
$$\sum_{u\in L_2}\sum_{w\in K_1\cup L_1\cup\{v\}} d(u,w) = 2l(1+2+3k+3(l-1)) = 6l(l+k).$$

Finally,

$$\sum_{\{u,w\}\subseteq K_1} d(u,w) = 2\binom{k}{2} = k(k-1), \qquad \sum_{\{u,w\}\subseteq L_1} d(u,w) = 2\binom{l}{2} = l(l-1),$$
$$\sum_{u\in K_1}\sum_{w\in L_1} d(u,w) = 2kl, \qquad \sum_{w\in K_1\cup L_1} d(v,w) = k+l.$$

By Claim 7,

$$\sum_{\{x,y\}\subseteq L_3} d(x,y) \le n_l\Big(3n_l - \frac{3n_l}{2l} - 1\Big)$$

and from Corollary 2.4 it follows that

$$\sum_{\{x,y\}\subseteq K_3} d(x,y) \le n_k\Big(3n_k - \frac{2n_k}{k} - 1\Big).$$

Hence,

$$W(T) \le 3(n_k+n_l)^2 + (9k+14l)(n_k+n_l) - \frac{2n_k^2}{k} - \frac{3n_l^2}{2l}$$
$$- 4n_k - 6n_l + 6k^2 + 15l^2 + 19kl - 2k - 6l.$$

Now we complete the proof of Theorem 3.4. Let

$$f(n_k,n_l) = 3(n_k+n_l)^2 + (9k+14l)(n_k+n_l) - \frac{2n_k^2}{k} - \frac{3n_l^2}{2l}$$
$$- 4n_k - 6n_l + 6k^2 + 15l^2 + 19kl - 2k - 6l.$$

We find the maximum of $f(n_k,n_l)$ subject to the constraint

$$n_k + n_l = n - 2k - 3l - 1 = a.$$

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Let $F(n_k, n_l, \lambda) = f(n_k, n_l) - \lambda(n_k + n_l - a)$. Then using $F_{n_k}(n_k, n_l, \lambda) = F_{n_l}(n_k, n_l, \lambda)$ we get $4n_k/k = 3n_l/l - 2$. Substituting $n_l = a - n_k$ yields $n_k = k(3a - 2l)/(3k + 4l)$, and then we obtain $n_l = 2l(2a + k)/(3k + 4l)$. It is easy to check that these values of n_k and n_l give the maximum of $F(n_k, n_l, \lambda)$. Hence $W(T)$ is at most

$$3a^2 + (9k + 14l)a - \frac{2k(3a - 2l)^2}{(3k + 4l)^2} - \frac{6l(2a + k)^2}{(3k + 4l)^2} - \frac{4k(3a - 2l)}{3k + 4l} - \frac{12l(2a + k)}{3k + 4l} + 6k^2 + 15l^2 + 19kl - 2k - 6l.$$

Consequently,

$$\frac{2k(3a - 2l)^2}{(3k + 4l)^2} + \frac{6l(2a + k)^2}{(3k + 4l)^2} = \frac{6a^2 + 2kl}{3k + 4l}$$

and

$$\frac{4k(3a - 2l)}{3k + 4l} + \frac{12l(2a + k)}{3k + 4l} = \frac{12a(k + 2l) + 4kl}{3k + 4l},$$

and, using $a = n - 2k - 3l - 1$,

$$W(T) \le 3n^2 - (3k + 4l)n - 6n + k - 2l + 3 - \frac{6(n^2 - 2kn - 2ln - 2n - 3l^2 - kl + 2k + 2l + 1)}{3k + 4l}.$$

Since by Claim 5, k and l are at most $O(n^{1/2})$,

$$\begin{aligned} W(T) &\le 3n^2 - (3k + 4l)n - 6n - \frac{6n(n - 2k - 2l - 2)}{3k + 4l} + O(n^{1/2}) \\ &= 3n^2 - (3k + 4l)n - 6n - \frac{6n(n - 2)}{3k + 4l} + 3n\left(1 + \frac{k}{3k + 4l}\right) + O(n^{1/2}). \end{aligned}$$

Let $b = 3k + 4l$ such that the expression above is maximal. Then

$$3n^2 - bn - 6n - \frac{6n(n - 2)}{b} + 3n\left(1 + \frac{k}{b}\right)$$

is maximised for $b = 3k$ (and $l = 0$). Now we need to find b such that

$$f(n, b) = 3n^2 - (b + 2)n - \frac{6n(n - 2)}{b}$$

is maximal. The partial derivative $f_b(n, b) = 0$ yields the value $b = \sqrt{6(n - 2)}$, which gives us the maximum of $f(n, b)$, that is,

$$\begin{aligned} 3n^2 - 2\sqrt{6(n - 2)}n - 2n &\le 3n^2 - 2\left(\sqrt{6n} - \frac{12}{\sqrt{6n}}\right)n - 2n \\ &= 3n^2 - 2\sqrt{6}n^{3/2} - 2n + O(n^{1/2}). \end{aligned}$$

Clearly $W(T) \le f(n, b) + O(n^{1/2})$.

It remains to prove that the upper bound is best possible. We show that there is an infinite family of trees T_1 such that

$$W(T_1) = 3n^2 - 2\sqrt{6}n^{3/2} - 2n + O(n^{1/2}).$$

Let $n = (3/2)k^2 + 1$ where k is even. Let T_1 be a tree of order n, diameter 6, with the central vertex v, where the degree of v is k, any vertex in $N(v)$ has one neighbour in $N_2(v)$, and any vertex in $N_2(v)$ is adjacent to $n = (3/2)k - 2 = (1/2)\sqrt{6(n-1)} - 2$ vertices in $N_3(v)$. Then $|N(v)| = |N_2(v)| = k = (1/3)\sqrt{6(n-1)}$ and

$$|N_3(v)| = n_k = k\Big(\frac{3}{2}k - 2\Big) = n - \frac{2}{3}\sqrt{6(n-1)} - 1.$$

We have

$$\sum_{\{y,x\}\subseteq N_3(v)} d(y, x) = n_k\Big(3n_k - \frac{2n_k}{k} - 1\Big),$$

which is the upper bound in Lemma 2.3 if the diameter is 6. Consequently we get equality in Claim 8 (where in our case $l = 0$ and $n_l = 0$). It follows that

$$W(T_1) = 3n_k^2 + 9kn_k - \frac{2n_k^2}{k} - 4n_k + 6k^2 - 2k.$$

Since $n_k = k(3k/2 - 2)$, we obtain $W(T_1) = (27/4)k^4 - 9k^3 + 6k^2 - 2k$ or equivalently

$$W(T_1) = 3n^2 - 2n\sqrt{6(n-1)} - 2n + \tfrac{4}{3}\sqrt{6(n-1)} - 1 = 3n^2 - 2\sqrt{6}n^{3/2} - 2n + O(n^{1/2}).$$

The proof is complete. □

Since by (1.1) and (1.2), $D'(T) = 4W(T) - n(n-1)$ and $\mathrm{Gut}(T) = 4W(T) - (2n - 1)(n-1)$, we obtain the following corollaries.

Corollary 3.5. *Let T be a tree of order n and diameter d. Then the degree distance $D'(T)$ is at most:*

(i) $4n^2 - 11n + 12$ *if* $d = 3$;
(ii) $7n^2 - 8n\sqrt{n-1} - 11n + 8\sqrt{n-1} + 4$ *if* $d = 4$;
(iii) $8n^2 - 8n^{3/2} + O(n)$ *if* $d = 5$;
(iv) $11n^2 - 8\sqrt{6}n^{3/2} - 7n + O(n^{1/2})$ *if* $d = 6$.

Corollary 3.6. *Let T be a tree of order n and diameter d. Then the Gutman index $\mathrm{Gut}(T)$ is at most:*

(i) $3n^2 - 9n + 11$ *if* $d = 3$;
(ii) $6n^2 - 8n\sqrt{n-1} - 9n + 8\sqrt{n-1} + 3$ *if* $d = 4$;
(iii) $7n^2 - 8n^{3/2} + O(n)$ *if* $d = 5$;
(iv) $10n^2 - 8\sqrt{6}n^{3/2} - 5n + O(n^{1/2})$ *if* $d = 6$.

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