On inverse Wiener interval problem of trees

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Abstract

The Wiener index $W(G)$ of a simple connected graph $G$ is defined as the sum of distances over all pairs of vertices in a graph. We denote by $W[T_n]$ the set of all values of Wiener index for a graph from the class $T_n$ of trees on $n$ vertices. The largest interval of contiguous integers (contiguous even integers in case of odd $n$) contained in $W[T_n]$ is denoted by $W^{int}[T_n]$. In this paper we prove that both sets are of cardinality $\frac{1}{6}n^3 + O(n^2)$ in the case of even $n$, while in the case of odd $n$ we prove that the cardinality of both sets equals $\frac{1}{12}n^3 + O(n^2)$ solving thus two conjectures posed in literature.

Keywords: Wiener index, Wiener inverse interval problem, Tree.

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1 Introduction

The Wiener index of a connected graph $G$ is defined as the sum of distances over all pairs of vertices, i.e.

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

It was first introduced in [9] and it was used for predicting the boiling points of paraffins. Since the index was very successful many other topological indices were introduced later which use distance matrix of a graph. There is a recent survey by Gutman et al. [6] in which finding extremal values and extremal graphs for the Wiener index and several of its variations is nicely presented. Given the class of all simple connected graphs on $n$ vertices it is easy to establish extremal graphs for the Wiener index, those are complete graph $K_n$ and path $P_n$. The same holds for the class of tree graphs on $n$ vertices in which minimal tree is the star $S_n$ and the maximal tree is path $P_n$. Many other bounds on Wiener index are also established in literature.

In [2] Gutman and Yeh proposed the inverse Wiener index problem, i.e. for a given value $w$ the problem of finding a graph (or a tree) $G$ for which $W(G) = w$. The first attempt at solving the problem was made in [5] where integers up to 1206 were checked and 49 integers were found that are not Wiener indices of trees. In [1] it was computationally proved that for all integers $w$ on the interval from $10^3$ to $10^6$ there exists a tree with Wiener index $w$. The problem was finally fully solved in 2006 when two papers were published solving the problem independently. It was proved in [8] that for every integer $w > 108$ there is a caterpillar tree $G$ such that $W(G) = w$. The other
proof is from the paper [7] where it was proved that all integers except those 49 are Wiener indices of trees with diameter at most 4.

A related question is to ask what value of the Wiener index can a graph (or a tree) \( G \) on \( n \) vertices have? In order to clarify further this problem one may also ask how many such values are there, how are they distributed along the related interval or how many of them are contiguous. In [4] this problem is named the Wiener inverse interval problem (see also a nice recent survey [3] which covers the topic). In that paper the set \( W(G_n) \) is defined as the set of all values of Wiener index for graphs \( G \in \mathcal{G}_n \), where \( \mathcal{G}_n \) is a class of simple connected graphs on \( n \) vertices. Similarly, \( W[T_n] \) is defined as the set of values \( W(G) \) for all trees on \( n \) vertices (\( \mathcal{T}_n \) denotes the class of trees on \( n \) vertices). Also, \( W^{\text{int}}[\mathcal{G}_n] \) (or analogously \( W^{\text{int}}[\mathcal{T}_n] \)) is defined to be the largest interval of contiguous integers such that \( W^{\text{int}}[\mathcal{G}_n] \subseteq W[\mathcal{G}_n] \) (or analogously \( W^{\text{int}}[\mathcal{T}_n] \subseteq W[\mathcal{T}_n] \)). In [4] the Wiener inverse interval problem on class \( \mathcal{G}_n \) was considered, while for the same problem on \( \mathcal{T}_n \) following two conjectures were made.

Conjecture 1 The cardinality of \( W[\mathcal{T}_n] \) equals \( \frac{1}{6}n^3 + O(n^2) \).

Conjecture 2 The cardinality of \( W^{\text{int}}[\mathcal{T}_n] \) equals \( O(n^3) \).

In this paper we will consider these two conjectures. First, we will prove that for a tree \( G \) on odd number of vertices \( n \) the value \( W(G) \) can be only even number. That means that the inverse Wiener interval problem in that case has to be reformulated as the problem of finding the largest interval of contiguous even integers such that \( W^{\text{int}}[\mathcal{T}_n] \subseteq W[\mathcal{T}_n] \). Since \( |W[\mathcal{T}_n]| \leq W(P_n) - W(S_n) = \frac{1}{3}n^3 - n^2 + \frac{11}{3}n - 1 \), we now conclude that the cardinality of \( W[\mathcal{T}_n] \) in the case of odd \( n \) can be at most \( \frac{1}{12}n^3 + O(n^2) \). Given that reformulation, we will prove both conjectures to be true. Even more, we will prove the strongest possible version of Conjecture 2 by proving that \( |W^{\text{int}}[\mathcal{T}_n]| \) also equals \( \frac{1}{6}n^3 + O(n^2) \) (i.e. \( \frac{1}{6}n^3 + O(n^2) \) in case of odd \( n \)) which is the best possible result given the upper bound on \( |W[\mathcal{T}_n]| \) derived from \( W(P_n) - W(S_n) \).

The present paper is organised as follows. It the next section basic definitions and preliminary results are given. In the third section the problem is solved for trees on even number of vertices, while in the fourth section the problem is solved for trees on odd number of vertices.

2 Preliminaries

Let \( G = (V(G), E(G)) \) be a simple connected graph having \( n = |V(G)| \) vertices and \( m = |E(G)| \) edges. For a pair of vertices \( u, v \in V(G) \) we define the distance \( d_G(u, v) \) as the length of the shortest path connecting \( u \) and \( v \) in \( G \). For a vertex \( u \in V \) the degree \( \delta_G(u) \) is defined as the number of neighbors of vertex \( u \) in graph \( G \). When it doesn’t lead to confusion we will use abbreviated notation \( d(u, v) \) and \( \delta(u) \). Also, for a vertex \( u \in V(G) \) and a set of vertices \( A \subseteq V(G) \) we will denote \( d(u, A) = \sum_{v \in A} d(u, v) \). We say that a vertex \( u \in V(G) \) is a leaf if \( \delta_G(u) = 1 \), otherwise we will say that \( u \) is interior vertex of a graph \( G \). We say that a vertex \( u \in V(G) \) is a petal if it has a leaf for a neighbor. A graph \( G \) which does not contain cycles is called a tree. We say that a tree \( G \) is a caterpillar tree if all its interior vertices induce a path. Such path will be called interior path of a caterpillar. Let \( a \) and \( b \) be positive integers such that \( a \leq b \). We say that the interval \([a, b] \) is Wiener \( p \)--complete if there is a tree \( G \) in \( \mathcal{T}_n \) such that \( W(G) = a + pi \) for every \( i = 0, \ldots, \left\lfloor \frac{b-a}{p} \right\rfloor \). We say that the interval \([a, b] \) is Wiener complete if it is Wiener \( 1 \)--complete.

Let us now prove that the value of the Wiener index for a tree on odd number of vertices is even number.
Theorem 3 Let $G$ be a tree on odd number of vertices $n \geq 3$. Then $W(G)$ is even number.

Proof. The proof is by induction on $n$. The only tree on $n = 3$ vertices is $P_3$ for which it holds that $W(P_3) = 4$ which is even number. Let $G$ be a tree on $n > 3$ vertices where $n$ is an odd integer. Note that $G$ has at least two leaves $u_1$ and $u_2$ which are neighboring to petals $v_1$ and $v_2$ (it can happen $v_1 = v_2$). Let $G'$ be a tree on $n - 2$ vertices obtained by deleting leaves $u_1$ and $u_2$. By induction hypothesis we know that $W(G')$ is even number. Now, note that

$$W(G) = W(G') + d(u_1, V') + d(u_2, V') + d(u_1, u_2)$$

where $V' = V(G')$. Let $P$ be the path connecting vertices $v_1$ and $v_2$ in $G'$. For any vertex $v \in V'$ let $w$ be the vertex on $P$ which is closest to $v$ (i.e. $d(v, w) = \min\{d(v, x) : x \in V(P)\}$). Note that $d(v, v_1) + d(v, v_2) = 2d(v, w) + d(w, v_1) + d(w, v_2) = 2d(v, w) + d(v_1, v_2)$. We now distinguish two cases.

CASE I. Suppose $d(v_1, v_2)$ is even. In that case $d(v, v_1) + d(v, v_2)$ is even for every $v \in V'$ which implies $d(v, v_1) + d(v, u_2) = d(v, v_1) + 1 + d(v, v_2) + 1$ is also even for every $v \in V'$. Therefore $d(u_1, V') + d(u_2, V')$ must also be even. Further note that $d(u_1, u_2) = d(v_1, v_2) + 2$ is also even in this case. Since $W(G')$ is even by induction hypothesis, we conclude that $W(G)$ must be even too.

CASE II. Suppose $d(v_1, v_2)$ is odd. Then $d(v, v_1) + d(v, v_2)$ is odd for every $v \in V'$ which further implies $d(v, u_1) + d(v, u_2)$ is also odd for every $v \in V'$. Since there is odd number of vertices in $V'$, we conclude that $d(u_1, V') + d(u_2, V')$ must also be odd number. Also, note that $d(u_1, u_2) = d(v_1, v_2) + 2$ is also odd because $d(v_1, v_2)$ is odd. Therefore, $d(u_1, V') + d(u_2, V') + d(u_1, u_2)$ is a sum of two odd numbers and therefore must be even. Since $W(G')$ is even, we now conclude that $W(G)$ must be even.

The main tool for obtaining our results throughout the paper will be a transformation of a tree which increases the value of Wiener index by exactly four. We will call it Transformation A, but let us introduce its formal definition.

Definition 4 Let $G$ be a tree and $u \in V(G)$ a vertex of degree 4 such that neighbors $v_1$ and $v_2$ of $u$ are leaves, while neighbors $v_1$ and $v_2$ of $u$ are not leaves. We say that a tree $G'$ is obtained from $G$ by Transformation $A$ if $G'$ is obtained from $G$ by deleting edges $w_1$ and $w_2$, while adding edges $w_1v_1$ and $w_2v_2$.

Theorem 5 Let $G$ be a tree and $G'$ be a tree obtained from $G$ by Transformation A. Then $W(G') = W(G) + 4$.

Proof. For the simplicity sake we will use notation $d'(u, v)$ for $d_{G'}(u, v)$. Let $G_{w_i} = (V_{w_i}, E_{w_i})$ be the connected component of $G \setminus \{u\}$ which contains vertex $w_i$ for $i = 1, 2$. Note that the only distances that change in Transformation A are distances from vertices $v_1$ and $v_2$. For every $v \in V_{w_1} \cup V_{w_1}$ we have

$$d'(v_1, v) - d(v_1, v) + d'(v_2, v) - d(v_2, v) = 0.$$

For the vertex $u$ we have

$$d'(v_1, u) - d(v_1, u) + d'(v_2, u) - d(v_2, u) = 2.$$

Finally, we also have $d'(v_1, v_2) - d(v_1, v_2) = 2$. Therefore, $W(G') - W(G) = 4$ which proves the theorem.
Although Transformation A can be applied on any tree graph, we will mainly apply it on caterpillar trees. Moreover, it is critical to find a kind of caterpillar tree on which Transformation A can be applied repeatedly as many times as possible. For that purpose, let us prove the following theorem.

**Theorem 6** Let $G$ be a caterpillar tree and $P = u_1 \ldots u_d$ its interior path. If there is a vertex $u_i \in P$ of degree 4 such that $u_{i+j}$ is of degree 3 for every $j = 1, \ldots, k - 1$, than the interval $[W(G), W(G) + 4k^2]$ is Wiener $4$-complete.

**Proof.** By applying repeatedly Transformation A on exactly one vertex from $1$ each transformation the value of Wiener index will increase by $4$.

Note that for $k = O(n)$ different values of $d$ for which $k = O(n)$, we obtain roughly $O(n^3)$ graphs with different values of Wiener index which is exactly the result we aim at. So, that is what we are going to do in following sections, but in order to do that precisely we will have to construct four different special types of caterpillar trees. To easily construct those four types of caterpillar trees we first introduce two basic types of caterpillars from which those four types will be constructed by adding one or two vertices.

**Definition 7** Let $n, d$ and $x$ be positive integers such that $n \geq 18$ is even, $\left\lceil \frac{n-2}{4} \right\rceil \leq d \leq \frac{n-8}{2}$, and $x \leq \frac{d+4d-8n}{2}$. Caterpillar $B_1(n, d, x)$ is a caterpillar on even number of vertices $n$ obtained from path $P = u_0 \ldots u_{d-1}u_0u_1 \ldots u_d$ by appending a leaf to vertices $u_{d-1}$ and $u_d$ and by appending a leaf to $2k-1$ consecutive vertices $u_{-(k-1)}, \ldots, u_{k-1}$ where $k = \frac{n-(2d+1)-1}{2}$.

**Lemma 8** Let $n, d$ and $x$ be integers such that $B_1(n, d, x)$ is defined. Then

$$W(B_1(n, d, x)) = \frac{n^3}{3} + (-\frac{3d}{2} - \frac{5}{4})n^2 + (4d^2 + 10d + \frac{13}{3} - 2x)n + 2x^2 - \frac{8}{3}d^3 - 12d^2 - \frac{46d}{3} - 7.$$  

**Proof.** Note that for $k = \frac{n-(2d+1)-1}{2}$ and $x' = d - 1 + x$ we have

$$W(B_1(n, d, x)) = \sum_{i = -d}^{d} \sum_{j = i+1}^{d} (j - i) + \sum_{i = -(k-1)}^{k-1} \sum_{j = i+1}^{k-1} (j - i + 2) + (2d + 2 - 2(x - 1)) + \sum_{i = -d}^{d} \sum_{j = -(k-1)}^{k-1} (|i - j| + 1) + \sum_{i = -(k-1)}^{d} 2(|i - x'| + 1) + \sum_{i = -(k-1)}^{k-1} (2|i - x'| + 2).$$

Simplifying the expression yields the formula from the lemma statement.

**Definition 9** Let $n, d$ and $x$ be positive integers such that $n \geq 18$ is even, $4 \leq d \leq \left\lfloor \frac{n}{4} \right\rfloor$ and $x \leq \frac{n-4d+2}{2}$. Caterpillar $B_2(n, d, x)$ is a caterpillar on even number of vertices $n$ obtained from
path \(P = u_d \ldots u_1 u_0 u_1 \ldots u_d\) by appending a leaf to \(2k - 1\) consecutive vertices \(u_{-(k-1)}, \ldots, u_{k-1}\) where \(k = d - 1\), by appending \(x\) leaves to each of the \(u_{-(d-1)}\) and \(u_{(d-1)}\), and by appending \(r\) leaves to each of the \(u_{-d}\) and \(u_d\) where \(r = \frac{n - 4d - 2d + 2}{2} + 2\).

**Lemma 10** Let \(n, d\) and \(x\) be integers such that \(B_2(n, d, x)\) is defined. Then

\[
W(B_2(n, d, x)) = \left(\frac{d}{2} + 1\right)n^2 + \left(-2d - 2\right)n - \frac{8d^3}{3} + \frac{32d}{3} - 5 + 8x - 8dx - 2x^2.
\]

**Proof.** Let \(k = d - 1\) and \(r = \frac{n - 4d - 2d + 2}{2}\). Note that

\[
W(B_2(n, d, x)) = \sum_{i=-d}^{d} \sum_{j=i+1}^{d} (j - i) + \sum_{i=-(k-1)}^{k-1} \sum_{j=i+1}^{k-1} (j - i + 2) + 4\left(\frac{r}{2}\right) + x^2(2d) +
\]

\[
+ 4\left(\frac{r}{2}\right) + r^2(2d + 2) + \sum_{i=-d}^{d} \sum_{j=-(k-1)}^{k-1} (|i - j| + 1) +
\]

\[
+ 2x(3 + \sum_{i=3}^{2d+1} (i - 1)) + 2r \sum_{i=1}^{2d+1} i + 2x \sum_{i=-(k-1)}^{k-1} (i + d + 1)
\]

\[
+ 2r \sum_{i=-(k-1)}^{k-1} (i + d + 2) + 2(3xr + xr(2d + 1)).
\]

Simplifying this expression yields the desired formula. \(\blacksquare\)

Finally, let us denote \(d_1^{\text{min}} = \left\lceil \frac{n - 2}{4} \right\rceil\) and \(d_1^{\text{max}} = \frac{4 + 4d_1^{\text{min}} - n}{2}\), while \(d_2^{\text{max}} = \left\lfloor \frac{n}{4} \right\rfloor\). Note that

\[
B_1(n, d_1^{\text{min}}, x_1^{\text{max}}) = B_2(n, d_2^{\text{max}}, 1).
\]

### 3 Even number of vertices

**Definition 11** Let \(n, d\) and \(x\) be integers for which \(B_1(n - 2, d, x)\) is defined. For \(s = -1, 0, 1, 2\) caterpillar \(G_1(n, d, x, s)\) is a caterpillar on even number of vertices \(n\), obtained from \(B_1(n - 2, d, x)\) by appending a leaf to vertex \(u_s\) and a leaf to vertex \(u_d\) of path \(P = u_d \ldots u_1 u_0 u_1 \ldots u_d\) in \(B_1(n - 2, d, x)\).

**Lemma 12** Let \(n, d, x\) and \(s\) be integers for which \(G_1(n, d, x, s)\) is defined. Then

\[
W(G_1(n, d, x, s)) = W(B_1(n - 2, d, x)) + \frac{n^2}{4} + \frac{3n}{2} + 2d^2 + 3d + 2s^2 - s - 2x.
\]

**Proof.** Let \(k = \frac{(n - 2) - (2d + 1) - 1}{2}\), \(x' = -d - 1 + x\). We define function

\[
f(v) = \sum_{i=-d}^{d} (|v - i| + 1) + \sum_{i=-(k-1)}^{k-1} (|v - i| + 2) + (|x' - v| + 2 + |-x' - v| + 2)
\]

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Now, the definition of $G_1(n, d, x, s)$ implies
\[ W(G_1(n, d, x, s)) = W(B_1(n - 2, d, x)) + f(s) + f(d) + d - s + 2. \]
Plugging $s$ and $d$ into the formula for $f$ and simplifying the obtained formula yields the result.

As a direct consequence of Lemma 14, we obtain the following corollary.

**Corollary 13** It holds that
\[
\begin{align*}
W(G_1(n, d, x, 1)) &= W(G_1(n, d, x, 0)) + 1, \\
W(G_1(n, d, x, 2)) &= W(G_1(n, d, x, 0)) + 6, \\
W(G_1(n, d, x, -1)) &= W(G_1(n, d, x, 0)) + 3.
\end{align*}
\]

The main tool in proving the results will be Transformation A of the graph, which, for a given graph, finds another graph whose value of Wiener index is greater by 4. Therefore, it is critical to find a graph on which Transformation A can be applied consecutively as many times as possible. That was the basic idea behind constructing graph $G_1(n, d, x, s)$ as we did, so that we can use Theorem 14 in filling the interval between values $W(G_1(n, d, x, s))$ for consecutive values of $x$ and $d$.

So, let us first apply Theorem 14 (i.e. find the corresponding value of $k$) on the graph $G_1(n, d, x, s)$.

**Lemma 14** Let $n, d, x$ and $s$ be integers for which $G_1(n, d, x, s)$ is defined. For $k = \frac{1}{4}n - d - 4$ the interval $[W(G_1(n, d, x, s)), W(G_1(n, d, x, s)) + 4k^2]$ is Wiener 4-complete.

**Proof.** Let us denote $k_1 = \frac{(n - 2) - (2d + 1) - 1}{2}$. Note that $k_1$ is the half of the number of leaves appended to the vertices $u_{\pm j}$ of the interior path of $G_1(n, d, x, s)$ for $j = 0, \ldots, k - 1$. Since $s \leq 2$, note that the definition of $G_1(n, d, x, s)$ and Theorem 14 imply the result for $k = k_1 - 2$.

So, let us now establish for which values of $d$ the gap between $W(G_1(n, d, x, s))$ and $W(G_1(n, d, x - 1, s))$ is smaller than $4k^2$ which is a width of interval which can be filled by repeatedly applying Transformation A on $G_1(n, d, x, s)$ (i.e. by using Lemma 14).

**Lemma 15** Let $n, d, x \geq 2$ and $s$ be integers for which $G_1(n, d, x, s)$ is defined. For $d \leq \frac{1}{4}(n - \sqrt{2n - 8} - 8)$ the interval
\[ [W(G_1(n, d, x, s)), W(G_1(n, d, x - 1, s))] \]
is Wiener 4-complete.

**Proof.** First note that
\[ W(G_1(n, d, x - 1, s)) - W(G_1(n, d, x, s)) \leq W(G_1(n, d, 2, s)) - W(G_1(n, d, 1, s)) = 2(n - 5) + 2. \]

Therefore, Lemma 14 implies it is sufficient to find integers $n$ and $d$ for which it holds that $4k^2 \geq 2(n - 5) + 2$ where $k = \frac{1}{4}n - d - 4$. By simple calculation it is easy to establish that the inequality holds for $d \leq \frac{1}{2}(n - \sqrt{2n - 8} - 8)$ so the lemma is proved.

It is easy to show, using Lemma 14 that $W(G_1(n, d, x - 1, s)) - W(G_1(n, d, x, s)) = 2n - 4x$ which is divisible by 4 since $n$ is even. Therefore, Lemma 14 enables us to "glue" together Wiener 4-complete intervals
\[ [W(G_1(n, d, x, s)), W(G_1(n, d, x - 1, s))] \]
Definition 17 Let \( n, d \) and \( x \) be integers for which \( B_2(n - 2, d, x) \) is defined. For \( s = -1, 0, 1, 2 \) caterpillar \( G_2(n, d, x, s) \) is a caterpillar on even number of vertices \( n \), obtained from \( B_2(n - 2, d, x) \) by appending a leaf to vertex \( u_s \) and a leaf to vertex \( u_d \) of path \( P = u_{-d} \ldots u_{-1}u_0u_1 \ldots u_d \) in \( B_2(n - 2, d, x) \).

Lemma 18 Let \( n, d, x \) and \( s \) be integers for which \( G_2(n, d, x, s) \) is defined. Then

\[
W(G_2(n, d, x, s)) = W(B_2(n - 2, d, x)) + (2d + 4)n - 2d^2 - 7d - 6 - 2x + 2s^2 - s.
\]
Proof. Let \( k = d - 1 \) and \( r = \frac{n - 4d + 2}{2} \). We define function

\[
f(v) = \sum_{i=-d}^{d} (|v - i| + 1) + \sum_{i=-(k-1)}^{k-1} (|v - i| + 2) + x(|v + (d - 1)| + 2) + x(|v - (d - 1)| + 2) + r(|v + d| + 2) + r(|v - d| + 2).
\]

Now, the definition of \( G \) implies it is sufficient to find for which \( d \) such that

\[
W(G_2(n, d, x, s)) = W(B_2(n - 2, d, x)) + f(s) + f(d) + d - s + 2.
\]

Plugging \( s \) and \( d \) into the formula for \( f \) and simplifying the obtained formula yields the result. ■

Corollary 19 It holds that

\[
W(G_2(n, d, x, 1)) = W(G_2(n, d, x, 0)) + 1,
W(G_2(n, d, x, 2)) = W(G_2(n, d, x, 0)) + 6,
W(G_2(n, d, x, -1)) = W(G_2(n, d, x, 0)) + 3.
\]

As in the case of large \( d \), the main tool in obtaining the results will be the following lemma.

Lemma 20 Let \( n, d, x \) and \( s \) be integers for which \( G_2(n, d, x, s) \) is defined. For \( k = d - 3 \) the interval \([W(G_2(n, d, x, s)), W(G_2(n, d, x, s)) + 4k^2]\) is Wiener 4-complete.

Proof. Let us denote \( k_1 = d - 1 \). Note that \( k_1 \) is the half of the number of leafs appended to the vertices \( u_{\pm j} \) of the interior path of \( G_2(n, d, x, s) \) for \( j = 0, \ldots, k - 1 \). Since \( s \leq 2 \), note that the definition of \( G = G_2(n, d, x, s) \) and Theorem 3 imply the result for \( k = k_1 - 2 \) if \( s = 0 \).

We first use Lemma 21 to cover interval between \( W(G_2(n, d, x, s)) \) and \( W(G_2(n, d, x, -1, s)) \).

Lemma 21 Let \( n, d, x \geq 2 \) and \( s \) be integers for which \( G_2(n, d, x, s) \) is defined. For \( d \geq \frac{\sqrt{2}n - 8}{2} + 6 \) the interval

\[
[W(G_2(n, d, x, s)), W(G_2(n, d, x, -1, s))]
\]

is Wiener 4-complete.

Proof. First note that for \( x_{2}^{\max} = \frac{(n - 2) - 4d + 2}{2} \) it holds that

\[
W(G_2(n, d, x - 1, s)) - W(G_2(n, d, x, s)) \leq W(G_2(n, d, x_{2}^{\max} - 1, s)) - W(G_2(n, d, x_{2}^{\max}, s)) = 2(n - 5) + 2.
\]

Therefore, Lemma 21 implies it is sufficient to find for which \( n \) and \( d \) it holds that \( 4k^2 \geq 2(n - 5) + 2 \) where \( k = d - 3 \). By simple calculation it is easy to establish that the inequality holds for \( d \geq \frac{1}{2}(\sqrt{2}n - 8 + 6) \) so the theorem is proved. ■

Again, it is easy to show that \( W(G_2(n, d, x - 1, s)) - W(G_2(n, d, x, s)) = 4d + 4x - 8 \) which is divisible by 4. Therefore, using Lemma 21 we can again "glue" the interval for different values of \( x \) into
(one bigger interval which will be “roughly” Wiener complete when taking values of $W(G_2(n, d, x, s))$ for every $s = -1, 0, 1, 2$. The next thing is to cover the gap between $W(G_2(n, d - 1, 1, s))$ and $W(G_2(n, d, x_{2\text{max}}^n, s))$ which equals $n - 3$ plus the gap of 6 which arises from “rough” ends of Wiener complete interval for given $n$ and $d$.

**Lemma 22** Let $n, d, x_{2\text{max}}^n = \frac{(n - 2) - 4d + 2}{-2}$ and $s$ be integers for which $G_2(n, d, x_{2\text{max}}^n, s)$ and $G_2(n, d - 1, 1, s)$ is defined. For $d \geq \frac{1}{2}(\sqrt{n} + 3 + 8)$ the interval

$$[W(G_2(n, d - 1, 1, s)), W(G_2(n, d, x_{2\text{max}}^n, s)) + 6]$$

is Wiener 4-complete.

**Proof.** Since

$$W(G_2(n, d, x_{2\text{max}}^n, s)) + 6 - W(G_2(n, d - 1, 1, s)) = n + 3,$$

Lemma [20] implies it is sufficient to find $n$ and $d$ for which it holds that $4k^2 \leq n - 3$ where $k = (d - 1) - 3$. By simple calculation one obtains that inequality holds for $d \geq \frac{1}{2}(\sqrt{n} + 3 + 8)$ which proves the theorem. □

Therefore, using graphs $G_1(n, d, x, s)$ and $G_2(n, d, x, s)$ we obtained two big Wiener complete intervals, which it would be nice if we could “glue” together into one big Wiener complete interval. In order to do that, note that the equality (1) implies

$$G_2(n, d_{2\text{max}}^n, 1, s) = G_1(n, d_{1\text{min}}^\text{s}, x_{1\text{max}}^n, s)$$

for $d_{2\text{max}}^n = \frac{n - 2}{4}, d_{1\text{min}}^\text{s} = \frac{n - 4}{2}$ and $x_{1\text{max}}^n = \frac{4 + 4d_{1\text{min}}^\text{s} - (n - 2)}{2}$. Now we can state the theorem which is our main result.

**Theorem 23** Let $n \geq 30$, $d_{2\text{min}}^\text{s} = \frac{1}{2}(\sqrt{2n - 8} + 6)$, $x_{2\text{max}}^n = \frac{(n - 2) - 4d_{2\text{max}}^n + 2}{-2}$ and $d_{1\text{max}}^\text{s} = \frac{1}{2}(n - \sqrt{2n - 8} - 8)$. The interval

$$[W(G_2(n, d_{2\text{max}}^n, x_{2\text{max}}^n, -1)), W(G_1(n, d_{1\text{max}}^\text{s}, 1, 1))]$$

is Wiener complete.

**Corollary 24** For even $n \geq 30$ it holds that $|W[\mathcal{T}_n]| \geq |W^{\text{int}}[\mathcal{T}_n]| \geq \frac{1}{6}n^3 - \frac{1}{\sqrt{2}}n^{5/2} + O(n^2)$.

**Proof.** Using Theorem 23 and Lemmas 12 and 18 it is easy to calculate that

$$|W^{\text{int}}[\mathcal{T}_n]| \geq W(G_1(n, d_{1\text{max}}^\text{s}, 1, 1)) - W(G_2(n, d_{2\text{max}}^n, x_{2\text{max}}^n, -1)) =$$

$$= \frac{n^3}{6} - \frac{\sqrt{n^3 - n^4}}{\sqrt{2}} - 3n^2 + \frac{10}{3}\sqrt{2n^3 - 8n^2 + \frac{143n}{6}} + 25\sqrt{2n - 8} - 25.$$

□

We can now prove Conjectures 1 and 2 we stated in the introduction. Namely, since $|W^{\text{int}}[\mathcal{T}_n]| \leq |W[\mathcal{T}_n]| \leq W(P_n) - W(S_n) = \frac{1}{6}n^3 - n^2 + \frac{11}{6}n - 1$, then the following holds.

**Theorem 25** For even $n \geq 30$ it holds that $|W^{\text{int}}[\mathcal{T}_n]| = |W[\mathcal{T}_n]| = \frac{1}{6}n^3 + O(n^2)$. 

9
4 Odd number of vertices

**Definition 26** Let \( n, d \) and \( x \) be integers for which \( B_1(n-1, d, x) \) is defined. For \( s = 0, 1 \) caterpillar \( G_3(n, d, x, s) \) is a caterpillar on odd number of vertices \( n \), obtained from \( B_1(n-1, d, x) \) by appending a leaf to vertex \( u_s \) of path \( P = u_{-d} \ldots u_{-1}u_0u_1 \ldots u_d \) in \( B_1(n-1, d, x) \).

**Lemma 27** Let \( n, d, x \) and \( s \) be integers for which \( G_3(n, d, x, s) \) is defined. Then

\[
W(G_3(n, d, x, s)) = W(B_1(n-1, d, x)) + \frac{n^2}{4} - dn + 2d^2 + 5d + \frac{11}{4} - 2x + 2s^2.
\]

**Proof.** Let \( k = \frac{(n-1)-(2d+1)-1}{2} \), \( x' = -d + 1 + x \). The definition of \( G_3(n, d, x, s) \) implies

\[
W(G_3(n, d, x, s)) = W(B_1(n-1, d, x)) + \sum_{i=-d}^{d} (|s - i| + 1) +
\]

\[
+ \sum_{i=-(k-1)}^{k-1} (|s - i| + 2) + (s - x' + 2) +
\]

\[+ (-x' - s + 2).\]

Simplifying this expression yields the result. ■

As a direct consequence of Lemma 27 we obtain the following corollary.

**Corollary 28** It holds that \( W(G_3(n, d, x, 1)) = W(G_3(n, d, x, 0)) + 2 \).

We now want to apply Theorem 6 on \( G_3(n, d, x, s) \), i.e. establish the value of \( k \) in the case of this special graph.

**Lemma 29** Let \( n, d, x \) and \( s \) be integers for which \( G_3(n, d, x, s) \) is defined. For \( k = \frac{1}{2}n - d - \frac{5}{2} \) the interval \([W(G_3(n, d, x, s)), W(G_3(n, d, x, s)) + 4k^2]\) is Wiener 4-complete.

**Proof.** Let us denote \( k_1 = \frac{(n-1)-(2d+1)-1}{2} \). Note that \( k_1 \) is the half of the number of leafs appended to the vertices \( u_{\pm j} \) of the interior path of \( G_3(n, d, x, s) \) for \( j = 0, \ldots, k-1 \). Since \( s \leq 1 \), note that the definition of \( G_3(n, d, x, s) \) and Theorem 6 imply the result for \( k = k_1 - 1 \). ■

So, let us now establish for which values of \( d \) the gap between \( W(G_3(n, d, x, s)) \) and \( W(G_3(n, d, x-1, s)) \) is smaller than \( 4k^2 \) where \( k = \frac{1}{2}n - d - \frac{5}{2} \).

**Lemma 30** Let \( n, d, x \geq 2 \) and \( s \) be integers for which \( G_3(n, d, x, s) \) is defined. For \( d \leq \frac{1}{2}(n - \sqrt{2n - 6} - 5) \) the interval

\[ [W(G_3(n, d, x, s)), W(G_3(n, d, x-1, s))] \]

is Wiener 4-complete.

**Proof.** First note that

\[
G_3(n, d, x-1, s) - G_3(n, d, x, s) \leq G_3(n, d, 2, s) - G_3(n, d, 1, s) =
\]

\[= 2(n - 4) + 2.\]
Therefore, Lemma 29 implies it is sufficient to find integers \( n \) and \( d \) for which it holds that \( 4k^2 \geq 2(n - 4) + 2 \) where \( k = \frac{n}{4} - d - \frac{5}{2} \). By simple calculation it is easy to establish that the inequality holds for \( d \leq \frac{1}{2}(n - \sqrt{2n - 6} - 5) \) so the lemma is proved. ■

Using Lemma 27 it is easy to establish that

\[
W(G_3(n, d, x - 1, s)) - W(G_3(n, d, x, s)) = 2(n - 2x + 1)
\]

which is divisible by 4 since \( n \) is odd. Moreover, note that for \( x_{\text{max}}^3 = \frac{4 + 4d - (n-1)}{2} \) it holds that

\[
G_3(n, d, x_{\text{max}}^3, s) = G_3(n, d - 1, 1, s).
\]

Therefore we can use Lemma 30 and "glue" together intervals both on the border between \( x \) and \( x - 1 \) and on the border of \( d \) and \( d - 1 \), so we will obtain one large interval which is Wiener 2-complete (because of Corollary 25).

Again, here we have used \( G_3(n, d, x, s) \) to the maximum, but we have covered thus only caterpillars with large \( d \). Let us now use graph \( B_2(n, d, x) \) to create fourth special kind of caterpillars which we will use to widen our interval to caterpillars with small \( d \).

**Definition 31** Let \( n, d \) and \( x \) be integers for which \( B_2(n - 1, d, x) \) is defined. For \( s = 0, 1 \) caterpillar \( G_4(n, d, x, s) \) is a caterpillar on odd number of vertices \( n \), obtained from \( B_2(n - 1, d, x) \) by appending a leaf to vertex \( u_s \) of path \( P = u_{-d} \ldots u_{-1} u_0 u_1 \ldots u_d \) in \( B_2(n - 1, d, x) \).

**Lemma 32** Let \( n, d, x \) and \( s \) be integers for which \( G_4(n, d, x, s) \) is defined. Then

\[
W(G_4(n, d, x, s)) = W(B_2(n - 1, d, x)) + (2 + d)n - 2d^2 - 3d - 1 + 2s^2 - 2x.
\]

**Proof.** Let \( k = d - 1 \) and \( r = \frac{(n - 1) - 4d - 2x + 2}{2} \). The definition of \( G_4(n, d, x, s) \) implies

\[
W(G_4(n, d, x, s)) = W(B_2(n - 1, d, x)) + \sum_{i=-d}^{d} (|s - i| + 1) + \\
+ \sum_{i=-(k-1)}^{k-1} (|s - i| + 2) + (s - x' + 2) + \\
+ 2x(d + 1) + 2r(d + 2).
\]

Simplifying this expression yields the result. ■

**Corollary 33** It holds that \( W(G_4(n, d, x, 1)) = W(G_4(n, d, x, 0)) + 2 \).

Let us now apply Theorem 6 on \( G_4(n, d, x, s) \).

**Lemma 34** Let \( n, d, x \) and \( s \) be integers for which \( G_4(n, d, x, s) \) is defined. For \( k = d - 2 \) the interval \( [W(G_4(n, d, x, s)), W(G_4(n, d, x, s)) + 4k^2] \) is Wiener 4-complete.

**Proof.** Let us denote \( k_1 = d - 1 \). Note that \( k_1 \) is the half of the number of leafs appended to the vertices \( u_{\pm j} \) of the interior path of \( G_3(n, d, x, s) \) for \( j = 0, \ldots, k - 1 \). Since \( s \leq 1 \), note that the definition of \( G_4(n, d, x, s) \) and Theorem 6 imply the result for \( k = k_1 - 1 \). ■

Now we can establish the minimum value of \( d \) for which the difference between Wiener index of \( G_4(n, d, x, s) \) and \( G_4(n, d, x - 1, s) \) can be "covered" by Transformation A.
Lemma 35 Let \( n, d, x \geq 2 \) and \( s \) be integers for which \( G_4(n, d, x, s) \) is defined. For \( d \geq \frac{1}{2}(\sqrt{2n-6}+4) \) the interval
\[
[W(G_4(n, d, x, s)), W(G_4(n, d, x-1, s))]
\]
is Wiener 4-complete.

Proof. First note that for \( x_4^{\text{max}} = \frac{(n-1) - 4d + 2}{2} \) it holds that
\[
W(G_4(n, d, x, s)) - W(G_4(n, d, x, s)) \leq W(G_4(n, d, x_4^{\text{max}} - 1, s)) - W(G_4(n, d, x_4^{\text{max}}, s)) = 2(n - 4) + 2.
\]
Therefore, Lemma 34 implies it is sufficient to find integers \( n \) and \( d \) for which it holds that \( 4k^2 \geq 2(n-4) + 2 \) where \( k = d - 2 \). By simple calculation it is easy to establish that the inequality holds for \( d \leq \frac{1}{2}(n - \sqrt{2n-6} - 5) \) so the lemma is proved.

Using Lemma 32 it is easy to establish that
\[
W(G_4(n, d, x, s)) - W(G_4(n, d, s)) = 4(x + 2d - 2)
\]
which is divisible by 4. Moreover, note that for \( x_4^{\text{max}} = \frac{(n-1) - 4d + 2}{2} \) it holds that
\[
G_4(n, d, x_4^{\text{max}}, s) = G_4(n, d - 1, 1, s).
\]
Therefore we can use Lemma 33 and ”glue” together intervals both on the border between \( x \) and \( x - 1 \) and on the border of \( d \) and \( d - 1 \), so we will obtain one large interval which is Wiener 2-complete (because of Corollary 33).

Finally, noting that for \( d_3^{\text{min}} = \frac{n-3}{4}, x_3^{\max} = \frac{4 + 4d - (n-1)}{2} \) and \( d_3^{\max} = \frac{n-1}{4} \) it holds that
\[
G_3(n, d_3^{\text{min}}, x_3^{\max}, s) = G_4(n, d_4^{\text{max}}, 1, s),
\]
we conclude that we can ”glue” together two large Wiener 2-complete intervals we obtained (one for large values of \( d \) and the other for small values of \( d \)), and thus prove our main result.

Theorem 36 Let \( n \geq 21 \), \( d_3^{\text{max}} = \frac{1}{2}(n - \sqrt{2n-6} - 5) \), \( d_3^{\text{min}} = \frac{1}{2}(\sqrt{2n-6} + 4) \) and \( x_4^{\text{max}} = \frac{(n-1) - 4d_3^{\text{min}} + 2}{2} \) The interval
\[
[W(G_4(n, d_3^{\text{min}}, x_3^{\max}, 0)), W(G_3(n, d_3^{\max}, 1, 1))]
\]
is Wiener 2-complete.

Corollary 37 For odd \( n \geq 21 \) it holds that \( |W[T_n]| \geq |W^{\text{int}}[T_n]| \geq \frac{1}{12}n^3 - \frac{1}{2\sqrt{2}}n^{5/2} + O(n^2) \).

Proof. Using Theorem 23 and Lemmas 12 and 18 it is easy to calculate that
\[
|W^{\text{int}}[T_n]| \geq (W(G_3(n, d_3^{\text{max}}, 1, s)) - W(G_4(n, d_4^{\text{min}}, x_4^{\text{max}}, s)))/2 =
\]
\[
\frac{n^3}{12} - \frac{\sqrt{n^5 - 3n^4}}{2\sqrt{2}} - n^2 + \frac{5}{3} \frac{\sqrt{2n^3 - 6n^2}}{n^2} + \frac{83n}{12} + \frac{11}{6\sqrt{2}} - 13.
\]

We can now prove Conjectures 1 and 2 we stated in the introduction (to be more precise - prove the adjusted version of conjectures). Namely, Theorem 3 implies \( |W^{\text{int}}[T_n]| \leq |W[T_n]| \leq (W(P_n) - W(S_n))/2 = \frac{1}{12}n^3 - \frac{1}{2}n^2 + \frac{1}{2}n - \frac{1}{2} \). Therefore the following theorem is proved.

Theorem 38 For odd \( n \geq 21 \) it holds that \( |W^{\text{int}}[T_n]| = |W[T_n]| = \frac{1}{12}n^3 + O(n^2) \).
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