Some Remarks on Inverse Wiener Index Problem

Jiří Fink[1]*, Borut Lužar[2]†, Riste Škrekovski[2]‡

[1] Department of Applied Mathematics,
Faculty of Mathematics and Physics, Charles University
Malostranské náměstí 25, 118 00 Prague 1, Czech Republic
E-mail: fink@kam.mff.cuni.cz
[2] Institute of Mathematics, Physics, and Mechanics,
Jadranska 19, 1111 Ljubljana, Slovenia
E-mail: {borut.luzar, skrekovski}@gmail.com

Abstract

In 1995 Gutman and Yeh [3] conjectured that for every large enough integer w there exists a tree with Wiener index equal to w. The conjecture has been solved by Wang and Yu [8] and independently by Wagner [6]. We present a constant time algorithm to construct a tree with a given Wiener index. Moreover, we show that there exist $2^{\Omega(\sqrt[4]{w})}$ non-isomorphic trees with Wiener index w.

Keywords: Wiener index, Inverse Wiener index problem

1 Introduction

The sum of distances between all pairs of vertices $W(G)$ in a connected graph G as a graph invariant was first introduced by Wiener [9] in 1947. He observed a correlation between boiling points of paraffins and this invariant, which has later become known as Wiener index of a graph. Today, the Wiener index is one of the most widely used descriptors in chemical graph theory. Due to its strong connection to chemistry, where molecules have a tree-like structures, a lot of research was done on acyclic graphs (see [2] for survey).

In 1995 Gutman and Ye [3] considered an inverse Wiener index problem. They asked for which integers n there exist trees with Wiener index n, and posed the following conjecture:

Conjecture 1. *For all but finitely many integers n there exist trees with Wiener index n.*

Inspired by the conjecture above, Lepović and Gutman [4] checked integers up to 1206 and found 49 integers that are not Wiener indices of trees. In 2004, Ban, Bereg, and Mustafa [1] computationally proved that for all integers n on the interval from 10^3 to 10^8 there exist a tree with Wiener index n. Finally, in 2006, two proofs of the conjecture were published. First, Wang and Yu [8] proved that for every $n > 10^8$ there exists a caterpillar tree with Wiener

*Supported by project 1M0545 of the Czech Ministry of Education and Czech-Slovene bilateral project BI-CZ/10-11-004.

†Operation part financed by the European Union, European Social Fund.

‡Supported in part by ARRS Research Program P1-0297.

index n. The second result is due to Wagner [6], who proved that all integers but 49 are Wiener indices of trees with diameter at most 4.

In Section 2, we present a proof, similar to Wagner's, that we use to develop a constant time algorithm, which for a given, sufficiently large integer w returns a tree with diameter 4 and with Wiener index w in a constant number of arithmetic operations.

In Section 4, we prove that there exist at least $2^{\Omega(\sqrt[4]{w})}$ non-isomorphic trees with Wiener index w, i.e. there exist w_0 and $C > 0$ such that for every $w \geq w_0$ there are at least $2^{C\sqrt[4]{w}}$ trees with Wiener index w. On the other hand, note that the number of non-isomorphic trees with Wiener index w is at most $2^{\mathcal{O}(\sqrt{w})}$.

2 Inverse Wiener index problem for large values

Here, we present a proof of Conjecture 1, similar to Wagner's, for large values.

Let k, m and $s_1, \dots, s_k$ be non-negative numbers such that $m = \sum_{i=1}^k s_i$. Let $T_{s_1,\dots,s_k}$ be a tree that has one *center* vertex with k neighbours, called *branches*, and a branch i has other s_i neighbours, called *terminals*. Fig. 1 depicts the tree $T_{0,2,3,4}$. Note that $T_{s_1,\dots,s_k}$ has m terminals and $n = m + k + 1$ vertices. First, we compute the Wiener index of $T_{s_1,\dots,s_k}$.

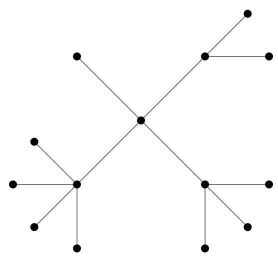

Figure 1: A tree $T_{0,2,3,4}$ with four branches and nine terminals.

Lemma 1.

$$W(T_{s_1,\dots,s_k}) = 2m^2 + (3k-1)m + k^2 - \sum_{i=1}^{k} s_i^2 \,.$$

Proof. We have three types of vertices (center, branch and terminal) and we compute the number of pairs of vertices of given type.

Type of vertices	distance	number of pairs of vertices
center – branch	1	k
center – terminal	2	m
branch – branch	2	$\binom{k}{2}$
branch – terminal	1	m
branch – terminal	3	$\sum_{i=1}^k (m - s_i)$
terminal – terminal	2	$\sum_{i=1}^k \binom{s_i}{2}$
terminal – terminal	4	$\frac{1}{2}\sum_{i=1}^k s_i(m - s_i)$

We sum up all products of the second and the third columns to obtain Wiener index of $T_{s_1,\dots,s_k}$. First, we sum up the last two rows separately.

$$2\sum_{i=1}^{k}\binom{s_i}{2}+4\cdot\tfrac{1}{2}\sum_{i=1}^{k}s_i(m-s_i)=\sum_{i=1}^{k}s_i^2-m+2m^2-2\sum_{i=1}^{k}s_i^2=2m^2-\sum_{i=1}^{k}s_i^2-m\,.$$

Now, we sum up all rows to obtain $W(T_{s_1,\dots,s_k})=2m^2+(3k-1)m+k^2-\sum_{i=1}^{k}s_i^2$. □

Since $\sum_{i=1}^{k}s_i$ and $\sum_{i=1}^{k}s_i^2$ have the same parity, the parity of $W(T_{s_1,\dots,s_k})$ depends only on the number of branches and terminals, thus moving terminals between branches does not change the parity. However, we obtain different Wiener indices by moving terminals between branches in $T_{s_1,\dots,s_k}$ with fixed number of vertices and branches. Our aim is to cover a long interval of numbers of the same parity by Wiener indices of $T_{s_1,\dots,s_k}$ with fixed k and m. Therefore, we need to know which values of $\sum_{i=1}^{k}s_i^2$ are obtained when the sum $\sum_{i=1}^{k}s_i$ equals m. The further computation is made simpler by restricting our attention on situation $0\le s_i\le s$ for all $i\in[k]$, where s is a fixed number and $[k]$ denotes the set $\{1,2,\dots,k\}$.

Lemma 2. *Let s, k and m be natural numbers such that $k\le m\le 2k$. Let $M_{\min}=3m-2k$ and $M_{\max}=s\left(m-\binom{s}{2}\right)$. For every z with the same parity as $M_{\min}$ and $M_{\min}\le z\le M_{\max}$ there exist $s_1,\dots,s_k\in\{0,\dots,s\}$ such that $\sum_{i=1}^{k}s_i=m$ and $\sum_{i=1}^{k}s_i^2=z$.*

Proof. We prove the statement by induction on z. The smallest value of $z=M_{\min}$ is obtained by choosing $s_1,\dots,s_{2k-m}=1$ and $s_{2k-m+1},\dots,s_k=2$.

Let us assume that $\sum_{i=1}^{k}s_i=m$ and $\sum_{i=1}^{k}s_i^2=z$ where $M_{\min}\le z\le M_{\max}-2$. We show how to obtain a sequence $\bar{s}_1,\dots,\bar{s}_k$ such that $\sum_{i=1}^{k}\bar{s}_i=m$ and $\sum_{i=1}^{k}\bar{s}_i^2=z+2$.

We will show that there exist two indices a and b such that $0<s_a=s_b<s$. Then, just let $\bar{s}_a=s_a-1$ and $\bar{s}_b=s_b+1$ and $\bar{s}_i=s_i$ for all other i and observe that the sequence $\bar{s}_1,\dots,\bar{s}_k$ satisfies our requirements.

So, if there are no such a and b, then every number of $[s-1]$ occurs at most once in the sequence $s_1,\dots,s_k$. Since $\sum_{i=1}^{k}s_i=m$, there exist at least

$$\left\lceil\frac{m-\sum_{i=1}^{s-1}i}{s}\right\rceil=\left\lceil\frac{m-\binom{s}{2}}{s}\right\rceil$$

indices i with $s_i=s$. But, this is impossible since

$$z=\sum_{i=1}^{k}s_i^2\ge s^2\left\lceil\frac{m-\binom{s}{2}}{s}\right\rceil\ge s\left(m-\binom{s}{2}\right)=M_{\max}\ge z+2\,.$$

□

Now, we present a short proof of the inverse Wiener index problem for large values.

Theorem 3. *For every sufficiently large number w there exists a tree T with Wiener index w.*

Proof. We put $m=k+1$ in order to make the computation simpler. Hence, using the notation of Lemma 2, we have $M_{\min}=k+3$ and $M_{\max}=s\left(k+1-\binom{s}{2}\right)$. By Lemma 1, it follows that $W(T_{s_1,\dots,s_k})=6k^2+6k+1-\sum_{i=1}^{k}s_i^2$. As the smallest value of $\sum_{i=1}^{k}s_i^2$ is $k+3$, we obtain that $W(T_{s_1,\dots,s_k}) \leq 6k^2 + 5k - 2$. Now, let k be the smallest number of the same parity as w that satisfies $w \leq 6k^2 + 5k - 2$. Let $z = 6k^2 + 6k + 1 - w$. Notice that z has the same parity as $M_{\min}$ and $z \geq M_{\min}$. If $z \leq M_{\max}$ then by Lemma 2 there exists a sequence $s_1, \dots, s_k$ such that $\sum_{i=1}^k s_i = m$ and $\sum_{i=1}^k s_i^2 = z$, and then by Lemma 1, the Wiener index of $T_{s_1,\dots,s_k}$ is w.

So, it only remains to prove the inequality $z \leq M_{\max}$. By the definition of z, we know $w = 6k^2 + 6k + 1 - z$, and by minimality of k we infer that $w > 6(k-2)^2 + 5(k-2) - 2$, which implies $25k - 11 > z$. We have to prove that $s\left(k - \binom{s}{2} + 1\right) \geq z$, and it suffices to prove $s\left(k - \binom{s}{2} + 1\right) \geq 25k - 11$, which we can simplify to $k(s-25) \geq \frac{1}{2}s^3 - \frac{1}{2}s^2 - s - 11$. Since w is sufficiently large, we can assume that $k \geq \frac{s^3 - s^2 - 2s - 22}{2(s-25)}$, where s is a fixed constant of size at least 26, and this establishes the theorem. □

3 Algorithm

Theorem 3 and Lemma 2 immediately give us the following algorithm which finds a tree with Wiener index w.

Algorithm 1

Require: Wiener index w that is large enough.
  $k \leftarrow$ The smallest number of the same parity as w that satisfies $w \leq 6k^2 + 5k - 2$.
  $m \leftarrow k + 1$
  $z \leftarrow 6k^2 + 6k + 1 - w$
  {Now, we find $s_1, \dots, s_k$ such that $0 \leq s_1, \dots, s_k \leq s$ and $\sum_{i=1}^k s_i = m$ and $\sum_{i=1}^k s_i^2 = z$.}
  $s_1, \dots, s_{k-1} \leftarrow 1$
  $s_k \leftarrow 2$
  {We start with $s_1, \dots, s_k$ satisfying $\sum_{i=1}^k s_i = m$ and the minimum value of $\sum_{i=1}^k s_i^2$ which we increase by 2 in every step.}
  while $\sum_{i=1}^k s_i^2 < z$ **do**
    Find two indices a and b such that $0 < s_a = s_b < s$.
    $s_a \leftarrow s_a - 1$
    $s_b \leftarrow s_b + 1$
  end while
Ensure: $W(T_{s_1,\dots,s_k}) = w$

We would like to achieve a constant time algorithm. However, there are two parts in Algorithm 1 which increase the time complexity. The first one is the while loop and the second part is searching for the indices a and b.

The second one can be handled easily: we store the number of branches having j terminals instead of the number of terminals of branch i. Let t_j be the number of indices $i \in [k]$ such that $s_i = j$. Since s is a constant, we can find $j \in \{0, \dots, s\}$ such that $t_j \geq 2$ in a constant time. Note that numbers $t_0, \dots, t_s$ uniquely describe $T_{s_1,\dots,s_k}$, so output of our algorithm is only $s + 1$ numbers.

Now, we describe how we speed up the while loop. For a given w we compute k, m, and z as described in Algorithm 1, and from them we create the required sequence $s_1, \dots, s_k$ in two steps.

In the first step, we compute α, β, and γ to be the number of branches with 0, 1, and s terminals, respectively. There remains $k' = k - \alpha - \beta - \gamma$ undefined numbers of the sequence.

The sum of undefined numbers must be $m' = m - \beta - s\gamma$; and the sum of squares of undefined numbers must be $z' = z - \beta - s^2\gamma$. In the second, we use Lemma 2 to find a sequence for the triple (k', m', z'). If we prove that all numbers of the new triple (k', m', z') are bounded by a constant, then the number of iterations in the while loop is bounded by a constant.

Let us recall our conditions:

$$\begin{aligned} k' &= k - \alpha - \beta - \gamma\,, \\ m' &= m - \beta - s\gamma\,, \\ z' &= z - \beta - s^2\gamma\,, \\ 3m' - 2k' \leq \quad z' &\leq s\left(m' - \binom{s}{2}\right)\,. \end{aligned}$$

Lemma 2 requires that the last inequality is satisfied. Note that the given triple (k, m, z) satisfies $3m - 2k \leq z \leq s\left(m - \binom{s}{2}\right)$ which is assured by the proof of Theorem 3.

Recall that $m = k + 1$. We keep the same relation also for m' and k', i.e. $m' = k' + 1$. This implies $\alpha = \gamma\,(s-1)$ and simplifies our conditions in the following way:

$$\begin{aligned} k' &= k - \beta - s\gamma\,, \\ z' &= z - \beta - s^2\gamma\,, \\ k' + 3 \leq \quad z' &\leq s\left(k' - \binom{s}{2} + 1\right)\,. \end{aligned} \tag{1}$$

Replacing the values of k' and z' in (1) gives us:

$$k - \beta - s\gamma + 3 \;\leq\; z - \beta - s^2\gamma \;\leq\; s\left(k - \beta - s\gamma - \binom{s}{2} + 1\right)\,,$$

which can be simplifed in the following way:

$$k - s\gamma + 3 \leq z - s^2\gamma \quad \text{and} \quad z - \beta \leq s\left(k - \beta - \binom{s}{2} + 1\right)\,.$$

Hence, we can easily solve the two inequalities independently. We choose the solutions:

$$\beta = \left\lfloor \tfrac{s(k+1)-z}{s-1} - \tfrac{s^2}{2} \right\rfloor \quad \text{and} \quad \gamma = \left\lfloor \tfrac{z-k-3}{s(s-1)} \right\rfloor\,.$$

It remains to show that we can bound all parameters k', m', and z' by a constant. From the definitions of k', β, and γ it follows that

$$\begin{aligned} k' &= k - \beta - s\gamma\,, \\ \beta + 1 &> \tfrac{s\left(k - \binom{s}{2} + 1\right) - z}{s-1}\,, \\ \gamma + 1 &> \tfrac{z-k-3}{s(s-1)}\,. \end{aligned}$$

It implies that k' is bounded by $\frac{s^2}{2} + s + \frac{2}{s-1}$ which is a constant. Hence, m' is also bounded since $m' = k' + 1$. Similarly, from $z' \leq s\left(k' - \binom{s}{2} + 1\right)$ it follows that z' is also bounded by a constant $s\left(\frac{3s}{2} + 1 + \frac{2}{s-1}\right)$. This analysis implies the following theorem:

Theorem 4. *The Algorithm 2 finds a tree with a given sufficiently large Wiener index in a constant time.*

Algorithm 2 Constant time algorithm for constructing tree of given Wiener index

Require: Wiener index w that is large enough.

{Specify a constant s that is used in calculations.}
$s \leftarrow 26$
{Compute k to be the smallest number of the same parity as w that satisfies $w \leq 6k^2 + 5k - 2$.}
$k \leftarrow \left\lceil \frac{\sqrt{24w+73}}{12} - \frac{5}{12} \right\rceil$
if $k \not\equiv w \pmod 2$ **then**
  $k \leftarrow k + 1$
end if
$m \leftarrow k + 1$
$z \leftarrow 6k^2 + 6k + 1 - w$
{Compute the number of branches with 0, 1 and s terminals that we obtain directly.}
$\beta \leftarrow \left\lfloor \frac{s(k+1)-z}{s-1} - \frac{s^2}{2} \right\rfloor$
$\gamma \leftarrow \left\lfloor \frac{z-k-3}{s(s-1)} \right\rfloor$
$\alpha \leftarrow \gamma(s-1)$
{Compute parameters for Lemma 2.}
$k' \leftarrow k - \alpha - \beta - \gamma$
$m' \leftarrow m - \beta - s\gamma$
$z' \leftarrow z - \beta - s^2\gamma$
{Base of induction in Lemma 2.}
$t_0, \ldots, t_s \leftarrow 0$
$t_1 \leftarrow k' - 1$
$t_2 \leftarrow 1$
{Initial sum of squares is $k' + 3$ and it is increased by 2 in every step.}
for $\frac{z'-k'-3}{2}$ times **do**
  Find index i such that $0 < i < s$ and $t_i \geq 2$. {A trivial loop over all indices.}
  {Move one terminal from a branch with i terminals into another branch with i terminals.}

  $t_{i-1} \leftarrow t_{i-1} + 1$
  $t_i \leftarrow t_i - 2$
  $t_{i+1} \leftarrow t_{i+1} + 1$
end for
{We add branches that were created in the beginning.}
$t_0 \leftarrow t_0 + \alpha$
$t_1 \leftarrow t_1 + \beta$
$t_s \leftarrow t_s + \gamma$

4 Semi-exponential number of trees with given Wiener index

In this section we prove that there exist at least $2^{\Omega(\sqrt[4]{w})}$ trees with Wiener index w. Here, let us mention that a tree with Wiener index w has at most $\lfloor \sqrt{w} \rfloor + 1$ vertices, since the Wiener index of the star S_n is $(n-1)^2$ and it is the smallest among all trees on n vertices. It is known that there are at most 3^n non-isomorphic trees on n vertices (see [5]), hence there are at most

$$\sum_{i=1}^{\lfloor\sqrt{w}\rfloor+1} 3^i = \tfrac{3}{2}(3^{\lfloor\sqrt{w}\rfloor+1} - 1)$$

non-isomorphic trees with at most $\sqrt{w}+1$ vertices. This proves the following proposition.

Proposition 5. *There is at most $2^{\mathcal{O}(\sqrt{w})}$ non-isomorphic trees with Wiener index w.*

In order to obtain many non-isomorphic trees with the same Wiener index w, we increase the maximum number of terminals on a branch to p, where $p = p(k)$ is a function of number of branches k. As described in the previous section, we denote a tree $T_{s_1,\dots,s_k}$ also by $T^*_{t_0,\dots,t_p}$, where t_i is the number of branches with precisely i terminals, for $i \in \{0, 1, \dots, p\}$. Let s be a fixed integer, and let $p > s$ be of the same parity as s. We show that for every combination of numbers t_j, where $j \in \mathcal{P} = \{s + 1, s + 3, \dots, p - 1\}$ and $t_j \in \{0, 1\}$, there exist numbers t_k, for $k \in \{0, 1, \dots, p\} \setminus \mathcal{P}$, such that $W(T^*_{t_0,\dots,t_p}) = w$. It is easy to see that all possible combinations of t_j, $j \in \mathcal{P}$, give exactly $2^{(p-s)/2}$ distinct sequences, i.e. non-isomorphic trees. Note that the numbers in $\mathcal{P}$ are of the same parity.

Next, let us introduce the notation used in this section. Let k_1, m_1, z_1, k_2, m_2, and z_2 be defined as

$$k_1 = \sum_{i=0}^{s} t_i\,, \qquad m_1 = \sum_{i=0}^{s} i\,t_i\,, \qquad z_1 = \sum_{i=0}^{s} i^2\,t_i\,,$$

$$k_2 = \sum_{i=s+1}^{p} t_i\,, \qquad m_2 = \sum_{i=s+1}^{p} i\,t_i\,, \qquad z_2 = \sum_{i=s+1}^{p} i^2\,t_i\,.$$

By the above definitions, the number of branches k, terminals m, and the sum of squares of numbers of terminals z, respectively, is

$$k = k_1 + k_2\,, \qquad m = m_1 + m_2\,, \qquad z = z_1 + z_2\,. \tag{2}$$

Now, we describe how to compute the undefined values of the sequence $\{t_i\}_{i=0}^{p}$, after the values t_j, $j \in \mathcal{P}$, are fixed. We want the number of branches with big number of terminals (at least $s+1$) to be always the same, so that the possible values of m_2 and z_2 are on a small interval. Therefore, we define $t_{i+1} = 1 - t_i$, where $i \in \mathcal{P}$. Hence, the value of k_2 is always equal to

$$k_2 = \tfrac{1}{2}(p - s)\,. \tag{3}$$

Note that the minimum (resp. maximum) values of m_2 and z_2 are obtained when for every $j \in \mathcal{P}$ holds that $t_j = 1$ (resp. $t_j = 0$). It is easy to see that the following inequalities hold:

$$\tfrac{1}{4}(p^2 - s^2) \leq \quad m_2 \quad \leq \tfrac{1}{4}(p\,(p+2) - s\,(s+2)) \tag{4}$$

$$\binom{p+1}{3} - \binom{s+1}{3} \leq \quad z_2 \quad \leq \binom{p+2}{3} - \binom{s+2}{3}\,. \tag{5}$$

Now, we present a variation of Lemma 2 in terms of t_i's.

Lemma 6. *Let s, k_1 and m_1 be natural numbers such that s is fixed and*

$$k_1 \leq m_1 \leq 2k_1\,. \tag{6}$$

Let $M_{\min} = 3m_1 - 2k_1$ and $M_{\max} = s\left(m_1 - \binom{s}{2}\right)$. For every integer z_1 with the same parity as $M_{\min}$ and

$$M_{\min} \leq z_1 \leq M_{\max} \tag{7}$$

there exist $t_0, \dots, t_s \in \{1, \dots, k_1\}$ such that $\sum_{i=0}^{s} t_i = k_1$, $\sum_{i=0}^{s} i\, t_i = m_1$, and $\sum_{i=0}^{s} i^2\, t_i = z_1$.

The equivalence between Lemmas 2 and 6 is obvious. Now, we are ready to state the main theorem of this section.

Theorem 7. *There exists a function $f(w) \in \Omega(\sqrt[4]{w})$ such that for every sufficiently large integer w there exist at least $2^{f(w)}$ trees with Wiener index w.*

Proof. In the proof we use the notation given above. We will prove that there exist at least $2^{(p-s)/2}$ non-isomorphic trees with sufficiently large Wiener index w, where $s = 124$ and p is a function of k_1 of order $\Omega(\sqrt[4]{w})$, defined as follows:

$$p = p(k_1) = \lfloor \sqrt{k_1} \rfloor - \left(\lfloor \sqrt{k_1} \rfloor \bmod 4\right). \tag{8}$$

Recall that k is of order $\mathcal{O}(\sqrt{w})$. Hence k_1 is also of order $\mathcal{O}(\sqrt{w})$, since $k = k_1 + \frac{1}{2}(p - s)$.

Let $t_i \in \{0, 1\}$, where $i \in \mathcal{P}$, be arbitrarily chosen, and set $t_{i+1} = 1 - t_i$. Observe that by this procedure all t_i, for $i \in \{s+1, s+2, \dots, p\}$ are fixed and so are k_2, m_2, and z_2. We will show that for every selection of t_i's, $i \in \mathcal{P}$, there exist numbers t_j, $j \in \{0, 1, \dots, s\}$, such that $k_1 = \sum_{i=0}^{s} t_i$, $m_1 = \sum_{i=0}^{s} i\, t_i$, and $z_1 = \sum_{i=0}^{s} i^2\, t_i$. Hence, the Wiener index of $T^*_{t_0,\dots,t_p}$ will be w. In order to do this, we need to satisfy the conditions of Lemma 6.

Let $m = 2k - 2$. From (2) it follows $m_1 + m_2 = 2(k_1 + k_2) - 2$. Hence,

$$m_1 = 2(k_1 + k_2) - 2 - m_2\,. \tag{9}$$

By Lemma 1, we have

$$w = W(T^*_{t_0,\dots,t_p}) = 15k^2 - 24k + 10 - z\,. \tag{10}$$

Note that (10) implies $z = 15k^2 - 24k + 10 - w$.

We proceed by showing that all the assumptions of Lemma 6 are satisfied. First, we show that the assumption (6) holds. By substituting m_2 in (9) with its minimum and maximum value derived in (4) and k_2 with its value derived in (3) we obtain the lower and upper bound for m_1:

$$m_1 \geq 2k_1 - \tfrac{1}{4}p^2 + \tfrac{1}{2}p + \tfrac{1}{4}s^2 - \tfrac{1}{2}s - 2\,, \tag{11}$$

$$m_1 \leq 2k_1 - \tfrac{1}{4}p^2 + p + \tfrac{1}{4}s^2 - s - 2\,. \tag{12}$$

Note that by the definition of p, the inequalities (11) and (12) imply that the assumption (6) of Lemma 6 is satisfied, since w is large enough.

Now, we show that we satisfy the assumption (7). First, note that by (5), we have the following lower bound for $z = z_1 + z_2$:

$$z \geq z_2^*, \tag{13}$$

where

$$z_2^* = \tfrac{1}{6}\big(p(k_1)^3 - p(k_1) - s^3 + s\big)\,.$$

Now, we compute the upper bound $M(k_1)$ that the Wiener index of $T^*_{t_0,\ldots,t_p}$ can achieve. We do this by substituting z in the equality (10) with its minimum value derived in (13). We also substitute k_2 by its value defined in (3).

$$\begin{aligned} M(k_1) &= 15(k_1+k_2)^2 - 24(k_1+k_2) + 10 - z_2^* \\ &= 15\left(k_1 + \tfrac{1}{2}(p(k_1)-s)\right)^2 - 24\left(k_1 + \tfrac{1}{2}(p(k_1)-s)\right) + 10 \\ &\quad - \tfrac{1}{6}\big(p(k_1)^3 - p(k_1) - s^3 + s\big) \end{aligned}$$

Let k_1 be the smallest integer of the same parity as w such that $M(k_1) \ge w$. By the choice of k_1, we also obtain the inequality

$$\begin{aligned} w \;>\; & 15\left((k_1-2) + \tfrac{1}{2}(p(k_1-2)-s)\right)^2 - 24\left((k_1-2) + \tfrac{1}{2}(p(k_1-2)-s)\right) + 10 \\ & - \tfrac{1}{6}\big(p(k_1-2)^3 - p(k_1-2) - s^3 + s\big)\,. \end{aligned} \tag{14}$$

Now, we apply the equality (10) to the inequality (14) using that $k = k_1 + k_2$ and obtain that

$$\begin{aligned} & 15\left(k_1 + \tfrac{1}{2}(p(k_1)-s)\right)^2 - 24\left(k_1 + \tfrac{1}{2}(p(k_1)-s)\right) + 10 - z_2 - z_1 > \\ & \quad 15\left((k_1-2) + \tfrac{1}{2}(p(k_1-2)-s)\right)^2 - 24\left((k_1-2) + \tfrac{1}{2}(p(k_1-2)-s)\right) + 10 \\ & \quad - \tfrac{1}{6}\big(p(k_1-2)^3 - p(k_1-2) - s^3 + s\big)\,. \end{aligned} \tag{15}$$

In order to simplify the calculations, we use the inequality

$$p(k_1) - p(k_1-2) \le 4\,. \tag{16}$$

It is easy to verify that (16) holds for every $k_1 \ge 4$. By plugging the inequality (16) in (15) we infer

$$\begin{aligned} z_1 \;<\; & 120k_1 + 60\sqrt{k_1} - 60s - 216 - z_2 \\ & + \tfrac{1}{6}\big(p(k_1-2)^3 - p(k_1-2) - s^3 + s\big)\,. \end{aligned} \tag{17}$$

Now we show that the assumption (7) of Lemma 6 is satisfied. The maximum value that z_1 attains, is obtained when z_2 is as small as possible. By replacing z_2 with its lower bound z_2^*, we infer

$$z_1 \;<\; 120k_1 + 60\sqrt{k_1} - 60s - 216 \le M_{\max}\,.$$

Since $s = 124$, the right side of assumption (7) of Lemma 6 is satisfied. On the other hand, the minimum value of z_1 is at least $M_{\min} = 3m_1 - 2k_1$, since

$$z_1 - M_{\min} \;=\; \sum_{i=0}^{s} i^2 t_i - \sum_{i=0}^{s} (3i-2)t_i = \sum_{i=0}^{s} (i-1)(i-2)t_i \ge 0\,.$$

Finally, we argue the parity condition of Lemma 6. First, note that k_2 (defined in (3)) is always even, since p and s are both divisible by 4. It follows that $k = k_1 + k_2$ has the same parity as w, since we chose k_1 to have the same parity as w. Using this fact and the equality (10) we have that z is even. Since $z = z_1 + z_2$, we infer that z_1 and z_2 have the same parity. Obviously, $z_2 = \sum_{i=s+1}^{p} i^2\, t_i$ and $m_2 = \sum_{i=s+1}^{p} i\, t_i$ also have the same parity. On the other hand, since $m = 2k - 2$, it follows that $m = m_1 + m_2$ is always even, implying that m_1 has the same parity as m_2. Now, m_1, m_2, z_1, and z_2 have the same parity, which implies that $M_{\min} = 3m_1 - 2k_1$ and z_1 are also of the same parity as required in Lemma 6.

Hence, we have satisfied all asuumptions of Lemma 6, therefore there exist t_j, $j \in \{0, 1, \ldots, s\}$, such that $W(T^*_{t_0,\ldots,t_p}) = w$ what completes the proof. □

References

[1] Y. A. Ban, S. Bereg, N. H. Mustafa, *On a conjecture on Wiener indices in combinatorial chemistry*, Algorithmica **40** (2004), 99–117.

[2] A. A. Dobrynin, R. Entringer, I. Gutman, *Wiener index of trees: theory and applications*, Acta Appl. Math. **66** (2001), 211–249.

[3] I. Gutman, Y. Yeh, *The sum of all distances in bipartite graphs*, Math. Slovaca **45** (1995), 327–334.

[4] M. Lepović, I. Gutman, *A collective property of trees and chemical trees*, J. Chem. Inf. Comput. Sci. **38** (1998), 823–826.

[5] R. Otter, *The Number of Trees*, Ann. Math. **49** (1948), 583–599.

[6] S. Wagner, *A class of trees and its Wiener index*, Acta Appl. Math. **91**(2) (2006), 119–132.

[7] S. Wagner, H. Wang, G. Yu, *Molecular graphs and the inverse Wiener index problem*, Discrete Appl. Math. **157** (2009), 1544–1554.

[8] H. Wang, G. Yu, *All but 49 numbers are Wiener indices of trees*, Acta Appl. Math. **92**(1) (2006), 15–20.

[9] H. Wiener, *Structural determination of paraffin boiling points*, J. Amer. Chem. Soc. **69** (1947), 17–20.