On Trees Having the Same Wiener Index as Their Quadratic Line Graph[☆]

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Abstract

We exhibit here some properties of trees T that satisfy the graph equation $W(L^2(T)) = W(T)$, where W(G) is the Wiener index of a graph G and L(G) is its line graph. In particular, we show that such trees may have arbitrarily many vertices of degree at least four, and that they may contain vertices whose degree exceeds six. These results disprove a recent conjecture of Knor, Škrekovski and Tepeh.

1 Introduction

The Wiener index of a graph is the sum of distances between all pairs of its vertices. It was suggested as a structural descriptor of acyclic organic molecules by Harry Wiener in 1947 [1], due to its high correlation with paraffin boiling points. Its relations to several further properties of organic molecules were subsequently discovered, and it is now widely used in quantitative structure-activity relationship studies (see, e.g., surveys [2–4]). Wiener index attracted attention of mathematicians in the late 1970s when it was introduced in graph theory under the names distance of a graph and transmission of a graph [5–7], and is further studied also in the form of average distance of graphs and networks [8,9]. Mathematical statements on Wiener index are mostly stated in the form of extremal results, which were recently surveyed in [15].

Let G be a graph with the vertex set V(G) and the edge set E(G). Cardinalities of V(G) and E(G) are called the order and the size of G, respectively. The line graph

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L(G) has the vertex set V(L(G)) = E(G), with two vertices of L(G) adjacent if and only if they share a vertex as edges of G. The iterated line graph $L^n(G)$ for a positive integer n is recursively defined as $L^n(G) = L(L^{n-1}(G))$, where $L^0(G) = G$. For majority of graphs, the size of $L^n(G)$ rapidly increases with n reflecting their branching and edge density. An accepted opinion in the mathematical chemistry community [10] is that it may be of interest to characterize molecular graphs by means of structural descriptors calculated for their derived structures. Iterated line graphs serve as good examples of derived structures, since their invariants have been already used for characterizing branching of acyclic molecular graphs [11], establishing partial order among isomeric structures [12], evaluating structural complexity of molecular graphs [13] and designing novel structural descriptors [14].

The graph equation $W(L^i(G)) = W(G)$ has raised considerable interest among graph theorists. Although there are solutions among general graphs for i=1 (surveyed in [16–18]), there exist no solutions among nontrivial trees, as Buckley [19] has shown that for trees $W(L(T)) = W(T) - \binom{n}{2}$. In the rest of the paper we focus our attention to trees. The case $i \geq 3$ for nontrivial trees has been resolved in a series of papers [20–26], where it is shown that $W(L^i(T)) = W(T)$ holds if and only if i=3 and T is isomorphic to a particular tree having two vertices of degree three only, with the remaining vertices of degree one or two.

Contrary to the cases i = 1 and $i \ge 3$, there exists a multitude of solutions of

$$W(L^2(T)) = W(T) \tag{1}$$

among trees. We denote by \mathcal{S} the set of all trees that are solutions of the equation (1). Trees in \mathcal{S} are enumerated up to 17 vertices in [3] and up to 26 vertices in [27]. A few infinite families of solutions are constructed earlier by Dobrynin and Mel'nikov [10,27–29] and by Knor and Škrekovski [30]. Solutions presented in these papers have very simple structure: they have at most four vertices of degree ≥ 3 and at most six pendent paths whose lengths can be arbitrarily large. This motivated Dobrynin and Mel'nikov [27] to pose the problem of finding an infinite family $\mathcal{F} \subset \mathcal{S}$ such that for any $n, m \in \mathbb{N}$ there exists a tree $T \in \mathcal{F}$ that has at least n pendent paths each having length at least m. Knor and Škrekovski [30] implicitly consider the set \mathcal{T} of trees without vertices of degree two such that $T' \in \mathcal{T}$ if and only if there exists $T \in \mathcal{S}$ that is homeomorphic to T' (i.e., T is a subdivision of T', so that T and T' have equally many vertices of any degree $\neq 2$). The small number of vertices of degree ≥ 3 in known solutions of (1) led Knor and Škrekovski to conjecture that the set \mathcal{T} is finite.

In [31] we provide both a positive answer to the Dobrynin-Mel'nikov problem and a negative answer to the Knor-Škrekovski conjecture by identifying a family of solutions of (1) that, for arbitrary $k, l \in \mathbb{N}$, contains trees with $\geq k$ vertices of degree three and with $\geq k$ pendent paths each of length $\geq l$. Motivated by our construction and previous findings, Knor, Škrekovski and Tepeh [18] further posed the following conjecture (as Conjecture 7.22 in [18]):

Conjecture 1 Trees from T satisfy the following:

- (a) no tree has a vertex of degree exceeding six;
- (b) there is a constant c such that no tree in \mathcal{T} has more than c vertices of degree ≥ 4 .

The purpose of this note is to disprove this conjecture by exhibiting in Section 2 another family of solutions of (1) that contains trees with an arbitrarily large number of vertices of degree four, and by providing in Section 3 exemplary solutions of (1) that contain vertices of degree larger than six. Some concluding remarks are given in Section 4.

2 Trees in \mathcal{T} with arbitrarily many degree 4 vertices

In our previous paper [31] we find an infinite family of solutions of (1) among quipus—trees that consist of a path with a new pendent path attached to each of its internal vertices. We continue our search here in a similarly defined class of trees.

Let n be a positive integer and let $h = \langle h_1, \ldots, h_n \rangle$ and $k = \langle k_1, \ldots, k_n \rangle$ be two vectors of positive integers. We define the quartic quipu Q(h,k) as follows. Let Q be the caterpillar consisting of a path $u_0u_1\cdots u_{n+1}$ and 2n pendent edges u_iv_i and u_iw_i for $i=1,\ldots,n$. Then Q(h,k) is obtained from Q by subdividing every edge u_iv_i , $i=1,\ldots,n$, to a path of length h_i and the edge u_iw_i to a path of length k_i . An example of a quartic quipu is shown in Figure 1 for illustration. These subdivided paths are called the cords of Q(h,k) and the path $u_0u_1\cdots u_{n+1}$ is called its main string. We assume without loss of generality that $h_i \geq k_i$ for each $i=1,\ldots,n$.

2.1 Wiener index of quartic quipu

The Wiener index of quartic quipu Q(h, k) and its quadratic line graph can be expressed in terms of n, h and k. By classifying pairs of vertices in Q(h, k) according to whether they belong to the main string or the cords, and by relying on the formula

$$W(P_t) = \frac{1}{6}(t-1)t(t+1)$$

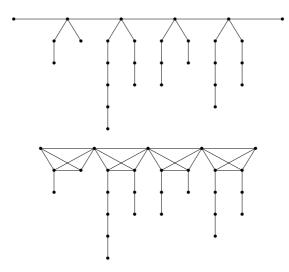


Figure 1: The quartic quipu Q(h,k) with $h=\langle 2,5,3,4\rangle$ and $k=\langle 1,3,2,3\rangle$ (top) and its line graph (bottom).

for the Wiener index of a path on t vertices [5], we obtain

$$W(Q(h,k)) = \frac{1}{6}(n+1)(n+2)(n+3)$$
(within the main string)
$$+ \sum_{i=1}^{n} \frac{1}{6}(h_{i}-1)h_{i}(h_{i}+1) + \sum_{i=1}^{n} \frac{1}{6}(k_{i}-1)k_{i}(k_{i}+1)$$
(within the cords)
$$+ \sum_{x=0}^{n+1} \sum_{i=1}^{n} \left[\sum_{y=1}^{h_{i}} (|x-i|+y) + \sum_{y=1}^{k_{i}} (|x-i|+y) \right]$$
(between the main string and the cords)
$$+ \sum_{1 \le i < j \le n} \left[\sum_{x=1}^{h_{i}} \sum_{y=1}^{h_{j}} (j-i+x+y) + \sum_{x=1}^{k_{i}} \sum_{y=1}^{k_{j}} (j-i+x+y) \right]$$
(between different cords)
$$+ \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{x=1}^{h_{i}} \sum_{y=1}^{k_{j}} (|j-i|+x+y).$$
(between different cords)

In order to compute the Wiener index of the quadratic line graph $L^2(Q(h,k))$ we sum the distances between pairs of edges of the line graph L(Q(h,k)). Using Figure 1 as a reference for descriptions, we have

$$\begin{split} W(L^2(Q(h,k))) &= \sum_{i=1}^n \sum_{j=1}^n 18(|j-i|+1) \\ & \text{(within and between the 4--cliques along the main string)} \\ &+ \sum_{i=1}^n \left[\frac{1}{6} h_i (h_i-1)(h_i-2) + \frac{1}{6} k_i (k_i-1)(k_i-2) \right] \\ & \text{(within the cords)} \\ &+ \sum_{x=1}^n \sum_{i=1}^n \left[\sum_{y=1}^{h_i-1} \left(6|x-i| + 6y + 3 \right) + \sum_{y=1}^{k_i-1} \left(6|x-i| + 6y + 3 \right) \right] \\ & \text{(between the main string and the cords)} \\ &+ \sum_{1 \leq i < j \leq n} \left[\sum_{x=1}^{h_i-1} \sum_{y=1}^{h_j-1} \left(j - i + x + y \right) + \sum_{x=1}^{k_i-1} \sum_{y=1}^{k_j-1} \left(j - i + x + y \right) \right] \\ & \text{(between different cords)} \\ &+ \sum_{j=1}^n \sum_{i=1}^n \sum_{x=1}^{h_i-1} \sum_{y=1}^{k_j-1} \left(|j-i| + x + y \right). \end{split}$$

After simplification, the above formulae for W(Q(h,k)) and $W(L^2(Q(h,k)))$ yield

(between different cords)

$$W(L^{2}(Q(h,k))) - W(Q(h,k)) = \frac{5}{2}n^{3} + 11n^{2} - \frac{9}{2}n - 1$$

$$+ \frac{1}{2}(3n^{2} + 2n - 4)\sum_{i=1}^{n}(h_{i} + k_{i}) - \left[\sum_{i=1}^{n}(h_{i} + k_{i})\right]^{2} + \frac{3n}{2}\sum_{i=1}^{n}(h_{i}^{2} + k_{i}^{2}) - 3\sum_{i=1}^{n}i(n - i + 1)(h_{i} + k_{i}).$$
(2)

2.2 Enumerating and mining the set of admissible pairs

It turns out that the set S of trees satisfying (1) contains plenty of quartic quipus. We say that two n-dimensional vectors h and k form an admissible pair if $Q(h,k) \in S$. The height of the pair (h,k) is equal to $\max\{h_1,\ldots,h_n,k_1,\ldots,k_n\}$. Using a brute force computer search, we enumerated admissible pairs of vectors with $n \leq 6$ and height at most 20 (assuming $h_i \geq k_i$ for each $i = 1,\ldots,n$). The resulting counts are presented in Table 1. There are no admissible pairs of vectors with $n \leq 6$ and height at most six. Increases of counts along the columns of Table 1 suggest that admissible pairs should exist for each $n \geq 3$ given a sufficiently large height.

Height	n = 3	n=4	n = 5	n = 6
7	2	0	0	0
8	18	0	0	0
9	15	4	0	0
10	86	248	0	0
11	131	522	69	0
12	175	2258	1610	0
13	259	5062	14245	56
14	327	10668	66303	26730
15	477	18916	231880	283940
16	638	33204	628512	2403602
17	734	51622	1443760	11426479
18	987	77456	3078456	42422052
19	1152	112642	5882413	125256913
20	1279	159974	10360898	328979427

Table 1: Numbers of admissible pairs of n-vectors of various fixed heights.

r	Admissible pairs	r	Admissible pairs
5	2	14	354
6	38	15	0
7	10	16	13976
8	0	17	1573160
9	0	18	23070982
10	0	19	20108286
11	770	20	7363860
12	18852	21	83 420
13	11032	22	134022298

Table 2: Numbers of admissible pairs (h, k) with n = 2r, $h_i \in \{4r, 4r + 1\}$ and $k_i = 4r$ for each i.

Regardless of the apparent abundance of admissible pairs, it is not at all straightforward to provide theoretical characterization of an infinite family of admissible pairs, due to the large number of variables appearing in (2). Fortunately, the number of admissible pairs remains plentiful even if we put appropriate restrictions on the structure of its vectors. A natural restriction is to assume that all cord lengths are equal to either a or a+1 for some a, in order for them to be as balanced as possible. Mining the set of available admissible pairs reveals that the choice

$$n = 2r, \quad a = 4r \tag{3}$$

ensures large number of admissible pairs, even with the additional assumption

$$k_i = 4r, \quad i = 1, \dots, n. \tag{4}$$

The numbers of such restricted admissible pairs for small r are shown in Table 2. Further mining for patterns among the admissible pairs of this type reveals that we can also assume the last r-2 components of h to be equal to 4r. Hence we assume for some subset of t coordinates $C = \{c_1, \ldots, c_t\} \subseteq \{1, 2, \ldots, r+2\}$ that

$$h_i = \begin{cases} 4r, & \text{if } i \in \{c_1, \dots, c_t\} \cup \{r+3, \dots, 2r\}, \\ 4r+1, & \text{otherwise.} \end{cases}$$
 (5)

An example of such admissible pair is

$$h = \langle 25, 25, 25, 25, 24, 24, 24, 25, 24, 24, 24, 24 \rangle$$

which corresponds to r = 6 and $C = \{5, 6, 7\}$.

Placing the above assumptions (3)-(5) in (2) we obtain in this case that $Q(h, k) \in \mathcal{S}$ if and only if

$$3\left[\sum_{i=1}^{t} c_i^2 - (2r+1)\sum_{i=1}^{t} c_i\right] = (2t-13)r^2 - 3(t+4)r - (t^2 - 6t + 3). \tag{6}$$

For t = 2 the above equation becomes

$$c_1^2 + c_2^2 - (2r+1)(c_1+c_2) = -3r^2 - 6r + \frac{5}{3}$$

which has no solutions as its left-hand side is an integer, while its right-hand side is not. For t=3 we found 467 solutions with $r \le 100$. For t=4 we found 1542 solutions with $r \le 100$. Those solutions with $r \le 20$ are listed in Table 3.

2.3 An infinite family of admissible pairs

We were able to identify among the enumerated solutions of (6) a few instances of a particular infinite family of admissible pairs, which we describe here. By setting

$$t = 4$$
 and $c_1 = 1$,

equation (6) simplifies to

$$(c_2^2 + c_3^2 + c_4^2) - (2r+1)(c_2 + c_3 + c_4) = -\frac{5r^2 + 18r - 5}{2},$$

				-				
r	$\{c_1,c_2,c_3\}$	r	$\{c_1,c_2,c_3\}$		r	$\{c_1, c_2, c_3, c_4\}$	r	$\{c_1, c_2, c_3, c_4\}$
6	{5,6,7}	15	{6,15,17}		5	{1,2,3,4}	17	{1,2,8,15}
6	$\{6,7,8\}$	15	$\{6,16,17\}$		5	$\{1,2,3,7\}$	17	$\{2,3,5,16\}$
9	$\{5,9,10\}$	15	$\{7,11,15\}$		11	$\{1,3,4,10\}$	17	$\{2,3,5,19\}$
9	$\{6,7,8\}$	15	$\{7,11,16\}$		11	$\{1,3,4,13\}$	17	$\{2,4,5,12\}$
9	$\{6,7,11\}$	15	{8,10,13}		13	{1,2,6,13}	17	${3,5,6,7}$
12	$\{6,10,11\}$	15	{9,10,11}		13	$\{1,2,6,14\}$	19	$\{1,2,10,14\}$
12	$\{6,10,14\}$	18	$\{7,15,17\}$		13	$\{1,3,5,11\}$	19	$\{1,4,7,14\}$
12	{7,8,12}	18	$\{7,15,20\}$		13	$\{1,4,6,7\}$	19	$\{2,4,5,16\}$
12	$\{7,8,13\}$	18	{8,13,16}		13	$\{2,3,4,10\}$	19	$\{2,4,8,10\}$
15	$\{6,14,15\}$	18	$\{9,11,18\}$		13	$\{2,3,5,8\}$	-	
15	{6,14,16}	18	${9,11,19}$	-				

Table 3: Solutions of equation (6) for $t \in \{3,4\}$ and $r \leq 20$.

and after completing the squares it becomes

$$(2r+1-2c_2)^2 + (2r+1-2c_3)^2 + (2r+1-2c_4)^2 = \frac{16r^2 - 36r + 29}{3}.$$
 (7)

Set further

$$c_2 = 2$$
,

and denote

$$p = 2r + 1 - 2c_3, \quad q = 2r + 1 - 2c_4.$$
 (8)

Equation (7) thus becomes

$$p^2 + q^2 = \frac{4r^2 + 2}{3}. (9)$$

Finally set

$$p = r \quad \Leftrightarrow \quad c_3 = \frac{r+1}{2}. \tag{10}$$

We will see in a moment that r will be odd, so that c_3 above is an integer. Equation (9) now simplifies to

$$r^2 - 3q^2 = -2, (11)$$

which is a particular case of Legendre's equation [32]. Legendre considered the equation

$$r^2 - dq^2 = \pm 2$$

in relation to the Pell's equation as it has smaller fundamental solutions. He showed that for all primes of the form d=4k+3 one case of the above equation has a solution: if d=8m+3 then $r^2-dq^2=-2$ is solvable, while if d=8m+7 then $r^2-dq^2=2$ is solvable.

In our particular case d = 3, the fundamental solution of (11) is

$$r_0 = 1, q_0 = 1,$$

while further solutions for $k \geq 1$ may be obtained as

$$r_k + q_k \sqrt{3} = \frac{(r_0 + q_0 \sqrt{3})^{2k+1}}{2^k} = \frac{(1 + \sqrt{3})^{2k+1}}{2^k}.$$
 (12)

To see why r_k and q_k as defined above are solutions of (11), note that for the conjugate surd we must have

$$r_k - q_k \sqrt{3} = \frac{(r_0 - q_0 \sqrt{3})^{2k+1}}{2^k} = \frac{(1 - \sqrt{3})^{2k+1}}{2^k},$$

so that

$$r_k^2 - 3q_k^2 = (r_k + q_k\sqrt{3})(r_k - q_k\sqrt{3}) = \frac{(1+\sqrt{3})^{2k+1}(1-\sqrt{3})^{2k+1}}{2^{2k}} = \frac{(-2)^{2k+1}}{2^{2k}} = -2.$$

From (12) we obtain

$$r_{k+1} + q_{k+1}\sqrt{3} = \frac{(1+\sqrt{3})^{2k+3}}{2^{k+1}} = (r_k + q_k\sqrt{3})\frac{(1+\sqrt{3})^2}{2},$$

which yields the recurrence relation

$$r_{k+1} = 2r_k + 3q_k,$$
 (13)
 $q_{k+1} = r_k + 2q_k.$

Since the fundamental solution $(r_0, q_0) = (1, 1)$ consists of two odd numbers, we see by induction that all further solutions (r_k, q_k) will consist of odd numbers as well, so that c_3 and c_4 in (8) and (10) above will be integers. Parameters of the first few admissible pairs produced in this way are given in Table 4.

Now we are in the position to disprove part (b) of Conjecture 1. Namely, it is evident from (13) that the sequence r_k tends to infinity with $k \to \infty$. Taking into account that the quartic quipu obtained from the admissible pair that corresponds to the solution (r_k, q_k) has $2r_k$ vertices of degree four, we see that the following theorem holds.

Theorem 1 For each real number c there exists a tree Q that has more than c vertices of degree four and satisfies $W(L^2(Q)) = W(Q)$.

r	q	c_1	c_2	c_3	c_4
5	3	1	2	3	4
19	11	1	2	10	14
71	41	1	2	36	51
265	153	1	2	133	189
989	571	1	2	495	704
3691	2131	1	2	1846	2626
13775	7953	1	2	6888	9799
51409	29681	1	2	25705	36569
191861	110771	1	2	95931	136476
716035	413403	1	2	358018	509334

Table 4: Parameters of the first ten admissible pairs obtained from the Legendre's equation.

3 Trees in \mathcal{T} with vertices of degree exceeding six

Here we present examples of trees $T \in \mathcal{S}$ and having vertices of degree larger than six, which disproves part (a) of Conjecture 1. Examples are found in a class of trees constructed similarly to quipus, by attaching cords to internal vertices of the main string. The difference is that the vertices on the main string may now have different numbers of cords attached to them. Such trees can be described by the sequence of cord lengths in linear order as they appear along the main string, with the convention that the lengths of multiple cords attached to the same main string vertex are grouped together in a pair of parentheses. We managed to find trees $T_7, T_8, T_9 \in \mathcal{S}$ which contain vertices of degrees 7, 8 and 9, respectively. Parameters and representations of these trees are listed in Table 5, while the tree T_7 is further illustrated in Figure 2.

Tree	Order	W(T)	Representation
T_7	603	9586262	(51, 54, 57, (51, 51, 53, 55, 57), 57, 53, 55)
T_8	1111	38502856	(62, 61, 62, 60, 61, 61, (60, 60, 60, 61, 62, 62), 60, 62, 60, 60, 62, 60)
T_9	2141	189643300	(75, 78, 78, 75, 80, 75, 78, 75, 79, 81, (75, 77, 79, 81, 81, 82, 82),
			76, 82, 79, 78, 81, 76, 81, 81, 77, 76)

Table 5: The trees $T_7, T_8, T_9 \in \mathcal{S}$ with maximum degree exceeding 6.

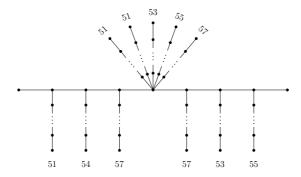


Figure 2: The tree T_7 . The number next to a cord indicates its length.

4 Conclusion

It can be observed from the findings that we presented in [31] and in this paper that there are many quipu-like trees T that satisfy the equation $W(L^2(T)) = W(T)$. Such admissible quipu-like trees remain plentiful even if reasonable further assumptions on their structure are made. In [31] we presented an infinite family of admissible quipus that contains trees with arbitrarily large number of vertices of degree three and trees with arbitrarily large number of pendent paths of arbitrarily large length. These findings positively answered a question of Dobrynin and Mel'nikov [27] and disproved a conjecture of Knor and Škrekovski [30]. Here we presented an infinite family of quartic quipus that contains trees with arbitrarily large number of vertices of degree four, as well as admissible quipu-like trees with vertices of degree exceeding six, thus disproving a conjecture of Knor, Škrekovski and Tepeh [18]. Experience from this study suggests that it is very likely that there exist admissible quipu-like trees with arbitrarily large vertex degrees, which we leave as a topic for further research. Moreover, abundance of solutions of $W(L^2(T)) = W(T)$ among quipu-like trees provides certain ground to believe that the second Knor-Skrekovski conjecture from [30] is correct, which claims that for each solution T of $W(L^2(T)) = W(T)$ there exist infinitely many other solutions that are homeomorphic to T.

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