Wiener index of generalized 4-stars and of their quadratic line graphs

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Abstract

We construct several infinite families of trees which have a unique branching vertex of degree 4 and whose Wiener index equals the Wiener index of their quadratic line graph. This solves an open problem of Dobrynin and Meľnikov.

Key words: Quadratic line graph, tree, Wiener index

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1   Introduction

We consider only finite, undirected, connected graphs without loops or multiple edges. Let G be a graph. By $V(G)$ and $E(G)$ we denote its vertex and edge sets, respectively. The sum of distances between all pairs of vertices of G is the *Wiener index $W(G)$*, that is,

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

Wiener index was introduced by Wiener in 1947, see [17]. This graph invariant belongs to the molecular structure-descriptors, called topological indices, that are

used for the design of molecules with desired properties, see e.g. [11], therefore it is widely studied by chemists. It attracted the attention of mathematicians in 1970's and it was reintroduced under the name of transmission and the distance of a graph, see [8] and [16]. Recently, several special issues of journals were devoted to (mathematical properties of) Wiener index, see [9] and [10]; for surveys see [3] and [4].

The *line graph* $L(G)$ of a graph G has vertices corresponding to the edges of G; two vertices being adjacent in $L(G)$ if and only if the corresponding edges have a common endvertex in G. The graph $L(L(G)) = L^2(G)$ is called the *quadratic line graph* of G and $L^t(G) = L(L^{t-1}(G))$ for $t \geq 3$. In [1], the following theorem was proved.

Theorem 1.1 *If T is a tree on n vertices, then $W(L(T)) = W(T) - \binom{n}{2}$.*

Thus, there is no tree with nonempty line graph for which $W(L(T)) = W(T)$ holds. However, there are trees T with property

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

see [2, 5, 6]. There is also a unique class of trees T with property $W(L^3(T)) = W(T)$, see [12]. However, for all trees on at least two vertices we have $W(L^i(T)) \neq W(T)$ for every $i \geq 4$, see [15] and also [13, 14]. Thus, the last unsettled case is the case of quadratic line graphs.

In [7] there are considered trees having a unique vertex of degree greater than 2. Such trees are called *generalized stars* (*starlike trees*). More precisely, *generalized t-star* is a tree obtained from the star $K_{1,t}$, $t \geq 3$, by replacing all its edges by paths of positive lengths. In [7] the following theorem is proved.

Theorem 1.2 *Let S be a generalized t-star with q edges and branches of length $k_1, k_2, \ldots, k_t$. Then,*

$$W(L^2(S)) = W(S) + \frac{1}{2}\binom{t-1}{2}\left(\sum_{i=1}^{t} k_i^2 + q\right) - q^2 + 6\binom{t}{4}. \tag{2}$$

Based on this theorem, it is proved in [7] that $W(L^2(S)) < W(S)$ if S is a generalized 3-star, and $W(L^2(S)) > W(S)$ if S is a generalized t-star where $t \geq 7$. Thus, property (1) can hold for generalized t-stars only when $t \in \{4, 5, 6\}$. In [7], for every $t \in \{4, 5, 6\}$ there are found several generalized t-stars with property (1), and for $t \in \{5, 6\}$ there are constructed infinite families of these generalized t-stars. The problem of existence of an analogous infinite family of generalized 4-stars is left open in [7]. In this paper we solve this problem and we construct several infinite families of generalized 4-stars with property (1). Hence, we can state the following theorem.

Theorem 1.3 *For every $t \in \{4, 5, 6\}$ there exist infinite families of generalized t-stars T with property (1). On the other hand, if $t \notin \{4, 5, 6\}$, $t \geq 3$, then there is no generalized t-star T with property (1).*

Two trees are homeomorphic if supressing all their vertices of degree 2 yields isomorphic trees. It is easy to find several mutually non-homeomorphic trees which all have property (1). However, we state here two conjectures.

Conjecture 1.4 *There exists a finite set of trees, $\mathcal{S}$, such that if a tree T has property (1) then T is homeomorphic to a tree from $\mathcal{S}$.*

Conjecture 1.5 *If a tree T has property (1), then there are infinitely many trees homeomorphic to T such that all these trees have property (1).*

2   The constructions

Let S be a generalized 4-star with branches of lengths k_1, k_2, k_3 and k_4. Suppose that $W(L^2(S)) = W(S)$. Then (2) is transformed to

$$2(k_1 + k_2 + k_3 + k_4)^2 = 3(k_1^2 + k_2^2 + k_3^2 + k_4^2) + 3(k_1 + k_2 + k_3 + k_4) + 12. \quad (3)$$

We present here three constructions yielding infinite sequences of quadruples (k_1, k_2, k_3, k_4) satisfying (3).

Construction 1. Solving (3) in k_4 gives

$$k_4 = \frac{4(k_1 + k_2 + k_3) - 3 \pm \sqrt{[3 - 4(k_1 + k_2 + k_3)]^2 + 4\rho}}{2},$$

where $\rho = 2(k_1 + k_2 + k_3)^2 - 3(k_1^2 + k_2^2 + k_3^3) - 3(k_1 + k_2 + k_3) - 12$. We have to choose k_1, k_2 and k_3 so that the square root will be an odd integer. The simplest choice is to set $\rho = 0$. Since k_4 cannot be 0, this choice implies $k_4 = 4(k_1 + k_2 + k_3) - 3$ and (3) reduces to $\rho = 0$, that is

$$2(k_1 + k_2 + k_3)^2 = 3(k_1^2 + k_2^2 + k_3^2) + 3(k_1 + k_2 + k_3) + 12. \quad (4)$$

Now we proceed analogously with k_3. Solving (4) in k_3 gives

$$k_3 = \frac{4(k_1 + k_2) - 3 \pm \sqrt{[3 - 4(k_1 + k_2)]^2 + 4\sigma}}{2},$$

where $\sigma = 2(k_1 + k_2)^2 - 3(k_1^2 + k_2^2) - 3(k_1 + k_2) - 12$. Setting $\sigma = 0$ implies $k_3 = 4(k_1 + k_2) - 3$ and (4) reduces to $\sigma = 0$, that is

$$k_1^2 + k_2^2 - 4k_1 k_2 + 3k_1 + 3k_2 + 12 = 0. \quad (5)$$

Since (5) is quadratic, for one k_1 there are two values of k_2 and vice-versa. Hence, we can construct a sequence $\{a_i\}_{i \in \mathbb{Z}}$, such that for every i, the pair (a_i, a_{i+1}) is a solution for (k_1, k_2) in (5).

For pairs (a_i, a_{i+1}) and (a_{i+1}, a_{i+2}), (5) transforms to

$$a_i^2 + a_{i+1}^2 - 4a_i a_{i+1} + 3a_i + 3a_{i+1} + 12 = 0 \tag{6}$$
$$a_{i+1}^2 + a_{i+2}^2 - 4a_{i+1} a_{i+2} + 3a_{i+1} + 3a_{i+2} + 12 = 0 \tag{7}$$

and subtracting (6) from (7) yields

$$a_{i+2}^2 - a_i^2 - 4a_{i+1}(a_{i+2} - a_i) + 3(a_{i+2} - a_i) = 0,$$

that is

$$(a_{i+2} + a_i)(a_{i+2} - a_i) - 4a_{i+1}(a_{i+2} - a_i) + 3(a_{i+2} - a_i) = 0. \tag{8}$$

Since we like to obtain different solutions, for fixed a_{i+1} we require $a_{i+2} \neq a_i$. Dividing (8) by $(a_{i+2} - a_i)$ results in a recurence relation

$$a_{i+2} - 4a_{i+1} + a_i + 3 = 0. \tag{9}$$

Since the roots of characteristic equation for (9) are $2 - \sqrt{3}$ and $2 + \sqrt{3}$, we have

$$a_i = c_1(2 - \sqrt{3})^i + c_2(2 + \sqrt{3})^i + c_3 \tag{10}$$

for suitable constants c_1, c_2 and c_3 depending on a_0 and a_1. Observe that quadruple $(4, 5, 33, 165)$ satisfies (3), $33 = 4(4 + 5) - 3$ and $165 = 4(4 + 5 + 33) - 3$. Thus, we may choose $a_0 = 4$ and $a_1 = 5$. Substituting (10) for $i = 0, 1, 2$ to (9) gives $c_3 = 3/2$ and consequently we can evaluate c_1 and c_2 from (10) when $i \in \{0, 1\}$. We get

$$a_i = \frac{5 + \sqrt{3}}{4}(2 - \sqrt{3})^i + \frac{5 - \sqrt{3}}{4}(2 + \sqrt{3})^i + \frac{3}{2}. \tag{11}$$

In Table 1 we present quadruples (a_i, a_{i+1}, k_3, k_4) for i, where $-3 \leq i \leq 3$.

...	$(a_{-3}, a_{-2}, k_3, k_4)$	$(a_{-2}, a_{-1}, k_3, k_4)$	(a_{-1}, a_0, k_3, k_4)
...	$(89, 25, 453, 2263)$	$(25, 8, 129, 645)$	$(8, 4, 45, 225)$

(a_0, a_1, k_3, k_4)	(a_1, a_2, k_3, k_4)	(a_2, a_3, k_3, k_4)	(a_3, a_4, k_3, k_4)	...
$(4, 5, 33, 165)$	$(5, 13, 69, 345)$	$(13, 44, 225, 1125)$	$(44, 160, 813, 4065)$	...

Table 1: Quadruples (a_i, a_{i+1}, k_3, k_4) for $i \in \{-3, -2, -1, 0, 1, 2, 3\}$.

By (11), $\lim_{i \to \infty} a_i = \infty$ (and also $\lim_{i \to -\infty} a_i = \infty$). Hence, we have an infinite sequence of quadruples $(a_i, a_{i+1}, 4a_i + 4a_{i+1} - 3, 20a_i + 20a_{i+1} - 15)$ satisfying (3) which solves the problem of Dobrynin and Mel'nikov. However, with a slight modification

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of the construction we can find many different infinite sequences of quadruples satisfying (3).

Construction 2. Another infinite sequences we can obtain from (4) when we fix k_1. Thus, set $k_1 = p$, to denote that k_1 is a parameter. Then (4) can be rewritten as

$$k_2^2 + k_3^2 - 4k_2k_3 + (3 - 4p)(k_2 + k_3) + p^2 + 3p + 12 = 0. \tag{12}$$

Since (12) is quadratic, similarly as above we can construct a sequence $\{a_i\}_{i\in\mathbb{Z}}$, such that for every i, the pair (a_i, a_{i+1}) is a solution for (k_2, k_3) in (12). Considering (12) for pairs (a_i, a_{i+1}) and (a_{i+1}, a_{i+2}), we get

$$a_{i+2}^2 - a_i^2 - 4a_{i+1}(a_{i+2} - a_i) + (3 - 4p)(a_{i+2} - a_i) = 0, \tag{13}$$

and dividing (13) by $(a_{i+2} - a_i)$ results in a recurence relation

$$a_{i+2} - 4a_{i+1} + a_i + 3 - 4p = 0. \tag{14}$$

Analogously as above, the roots of characteristic equation for (14) are $2 - \sqrt{3}$ and $2 + \sqrt{3}$ and an easy calculation shows that

$$a_i = \frac{\alpha + \beta\sqrt{3}}{12}(2 - \sqrt{3})^i + \frac{\alpha - \beta\sqrt{3}}{12}(2 + \sqrt{3})^i + \frac{3 - 4p}{2}, \tag{15}$$

where $\alpha = 6a_0 + 12p - 9$ and $\beta = 4a_0 - 2a_1 + 4p - 3$. (Observe that if p, a_0 and a_1 are integers, then by (14), every a_i is an integer number, $i \in \mathbb{Z}$.) In Table 2 we present a starting pair (a_0, a_1) for small values of p, $1 \le p \le 6$, such that the triple (p, a_0, a_1) satisfies (12), and also the explicit formula for a_i according to (15).

p	a_0	a_1	a_i
1	2	3	$\frac{1}{12}(15 + 3\sqrt{3})(2 - \sqrt{3})^i + \frac{1}{12}(15 - 3\sqrt{3})(2 + \sqrt{3})^i - \frac{1}{2}$
2	1	3	$\frac{1}{12}(21 + 3\sqrt{3})(2 - \sqrt{3})^i + \frac{1}{12}(21 - 3\sqrt{3})(2 + \sqrt{3})^i - \frac{5}{2}$
3	1	2	$\frac{1}{12}(33 + 9\sqrt{3})(2 - \sqrt{3})^i + \frac{1}{12}(33 - 9\sqrt{3})(2 + \sqrt{3})^i - \frac{9}{2}$
4	5	33	$\frac{1}{12}(69 - 33\sqrt{3})(2 - \sqrt{3})^i + \frac{1}{12}(69 + 33\sqrt{3})(2 + \sqrt{3})^i - \frac{13}{2}$
5	4	33	$\frac{1}{12}(75 - 33\sqrt{3})(2 - \sqrt{3})^i + \frac{1}{12}(75 + 33\sqrt{3})(2 + \sqrt{3})^i - \frac{17}{2}$
6	1	2	$\frac{1}{12}(69 + 21\sqrt{3})(2 - \sqrt{3})^i + \frac{1}{12}(69 - 21\sqrt{3})(2 + \sqrt{3})^i - \frac{21}{2}$

Table 2: Explicit formulae for given p, a_0 and a_1.

For these six values of p, quadruples (p, a_i, a_{i+1}, k_4) for i, where $-3 \le i \le 3$, are present in the following two tables.

i	$p = 1$	$p = 2$	$p = 3$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
-3	$(1, 87, 23, 441)$	$(2, 111, 28, 561)$	$(3, 206, 52, 1041)$
-2	$(1, 23, 6, 117)$	$(2, 28, 6, 141)$	$(3, 52, 11, 261)$
-1	$(1, 6, 2, 33)$	$(2, 6, 1, 33)$	$(3, 11, 1, 57)$
0	$(1, 2, 3, 21)$	$(2, 1, 3, 21)$	$(3, 1, 2, 21)$
1	$(1, 3, 11, 57)$	$(2, 3, 16, 81)$	$(3, 2, 16, 81)$
2	$(1, 11, 42, 213)$	$(2, 16, 66, 333)$	$(3, 16, 71, 357)$
3	$(1, 42, 158, 801)$	$(2, 66, 253, 1281)$	$(3, 71, 277, 1401)$
$\vdots$	$\vdots$	$\vdots$	$\vdots$

Table 3: Quadruples (p, a_i, a_{i+1}, k_4) for $p \in \{1, 2, 3\}$.

and

i	$p = 4$	$p = 5$	$p = 6$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
-3	$(4, 45, 8, 225)$	$(5, 69, 13, 345)$	$(6, 446, 112, 2253)$
-2	$(4, 8, 0, 45)$	$(5, 13, 0, 69)$	$(6, 112, 23, 561)$
-1	$(4, 0, 5, 33)$	$(5, 0, 4, 33)$	$(6, 23, 1, 117)$
0	$(4, 5, 33, 165)$	$(5, 4, 33, 165)$	$(6, 1, 2, 33)$
1	$(4, 33, 140, 705)$	$(5, 33, 145, 729)$	$(6, 2, 28, 141)$
2	$(4, 140, 540, 2733)$	$(5, 145, 564, 2853)$	$(6, 28, 131, 657)$
3	$(4, 540, 2053, 10305)$	$(5, 564, 2128, 10785)$	$(6, 131, 517, 2613)$
$\vdots$	$\vdots$	$\vdots$	$\vdots$

Table 4: Quadruples (p, a_i, a_{i+1}, k_4) for $p \in \{4, 5, 6\}$.

Observe that when $p \in \{4, 5\}$ then for $i \in \{-2, -1\}$ we have 0's in Table 4. The corresponding quadruples satisfy (3) but since they form generalized 3-stars instead of generalized 4-stars, the equation (3) cannot be applied to them. Hence, in these cases we have no solution. This failure is caused by the fact that although both c_1 and c_2 are positive in all the formulae in Table 2, c_3 is a negative constant. Consequently, it is obvious that in all the other cases we get positive quadrangles. Since $\lim_{i \to \infty} a_i = \infty$ in all the formulae in Table 2, we get another six infinite classes of generalized 4-stars S with $W(L^2(S)) = W(S)$. Observe that these classes can be combined. For instance, in Table 3 we see that $(1, 3, 11, 57)$ satisfies (3). Hence, we can set $p = 11$ and find another infinite sequence of quadruples satisfying (3).

Construction 3. In our first construction there is no number which is in all quadruples of the sequence, while in the second construction every sequence contains one number which is in all quadruples. In our last construction, every sequence contains

two numbers which are in all quadruples. Choose k_1 and k_2 to be constants, say p and r, respectively. Then (3) is transformed to

$$k_3^2 + k_4^2 - 4k_3k_4 + (3 - 4(p+r))(k_3 + k_4) + c = 0, \tag{16}$$

where c is a constant depending on p and r. Thus, there exists a sequence $\{a_i\}_{i \in \mathbb{Z}}$, such that for every i, the pair (a_i, a_{i+1}) is a solution for (k_3, k_4) in (16). Analogously as above we get a recurrence relation

$$a_{i+2} - 4a_{i+1} + a_i + 3 - 4(p+r) = 0, \tag{17}$$

and so

$$a_i = \frac{\alpha + \beta\sqrt{3}}{12}(2 - \sqrt{3})^i + \frac{\alpha - \beta\sqrt{3}}{12}(2 + \sqrt{3})^i + \frac{3 - 4(p+r)}{2}, \tag{18}$$

where $\alpha = 6a_0 + 12p + 12r - 9$ and $\beta = 4a_0 - 2a_1 + 4p + 4r - 3$. In Table 5 we present three starting pairs (a_0, a_1) for two pairs p and r, such that the quadruple (p, r, a_0, a_1) satisfies (3), and also the explicit formula for a_i according to (18).

p	r	a_0	a_1	a_i
1	2	3	21	$\frac{1}{12}(45 - 21\sqrt{3})(2 - \sqrt{3})^i + \frac{1}{12}(45 + 21\sqrt{3})(2 + \sqrt{3})^i - \frac{9}{2}$
4	5	9	72	$\frac{1}{12}(153 - 75\sqrt{3})(2 - \sqrt{3})^i + \frac{1}{12}(153 + 75\sqrt{3})(2 + \sqrt{3})^i - \frac{33}{2}$
4	5	33	165	$\frac{1}{12}(297 - 165\sqrt{3})(2 - \sqrt{3})^i + \frac{1}{12}(297 + 165\sqrt{3})(2 + \sqrt{3})^i - \frac{33}{2}$

Table 5: Explicit formulae for given p, r, a_0 and a_1.

For these three choices, quadruples (p, r, a_i, a_{i+1}) for i, where $-3 \leq i \leq 3$, are present in the following table.

i	$[1, 2, 3, 21]$	$[4, 5, 9, 72]$	$[4, 5, 33, 165]$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
-3	$(1, 2, 33, 6)$	$(4, 5, 84, 12)$	$(4, 5, 33, 0)$
-2	$(1, 2, 6, 0)$	$(4, 5, 12, -3)$	$(4, 5, 0, 0)$
-1	$(1, 2, 0, 3)$	$(4, 5, -3, 9)$	$(4, 5, 0, 33)$
0	$(1, 2, 3, 21)$	$(4, 5, 9, 72)$	$(4, 5, 33, 165)$
1	$(1, 2, 21, 90)$	$(4, 5, 72, 312)$	$(4, 5, 165, 660)$
2	$(1, 2, 90, 348)$	$(4, 5, 312, 1209)$	$(4, 5, 660, 2508)$
3	$(1, 2, 348, 1311)$	$(4, 5, 1209, 4557)$	$(4, 5, 2508, 9405)$
$\vdots$	$\vdots$	$\vdots$	$\vdots$

Table 6: Quadruples (p, r, a_i, a_{i+1}) determined by $[p, r, a_0, a_1]$.

When $(p, r) = (1, 2)$ then for $i \in \{-2, -1\}$ we have 0's in Table 6. Such 0's correspond to branches of length 0, which is impossible. In the case $(p, r) = (4, 5)$, when $(a_0, a_1) = (9, 72)$ then for $i \in \{-2, -1\}$ we get even negative numbers, and when $(a_0, a_1) = (33, 165)$ then we get 0's for $i \in \{-3, -2, -1\}$. This is caused by $c_3 < 0$. However, as c_1 and c_2 are positive in all the formulae in Table 5, in all the other cases we get positive lengths of branches. Hence, all the other quadruples generated by the way described above correspond to positive quadruples (k_1, k_2, k_3, k_4) satisfying (3). Since $\lim_{i \to \infty} a_i = \infty$ in all the formulae in Table 5, we get another three infinite classes of generalized 4-stars S with $W(L^2(S)) = W(S)$, although in the last case for nonnegative i we get the same quadruple as for $-i - 4$. Analogously as in the second construction, these classes can be combined to obtain arbitrarily many infinite sequences of quadruples satisfying (3).

The methods used in Constructions 1, 2 and 3 above do not work for generalized 5-stars and generalized 6-stars. For generalized 5-stars, solving (2) in k_5 gives $k_5 = (c \pm \sqrt{c^2 + \rho})/4$, so it is not enough to let $\rho = 0$. On the other hand, if one fixes k_1, k_2, k_3 and tries to find $\{a_i\}_{i \in \mathbb{Z}}$ so that $(k_1, k_2, k_3, a_i, a_{i+1})$ is a solution, then the recurrence relation is $2a_{i+2} - 2a_{i+1} + 2a_i + \sigma = 0$, where σ is an odd number. This forces a_i to be fractions. For generalized 6-stars, solving (2) in k_6 gives $k_6 = (c \pm \sqrt{c^2 + \rho})/8$, while for fixed k_1, k_2, k_3 and k_4 the recurrence relation is $4a_{i+2} - 2a_{i+1} + 4a_i + \sigma = 0$, where σ is odd.

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