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Trees, Quadratic Line Graphs and the Wiener Index

Andrey A. Dobrynin* and Leonid S. Mel'nikov*

Sobolev Institute of Mathematics, Siberian Branch of the Russian Academy of Sciences, Novosibirsk 630 090, Russia

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The Wiener index is a topological index defined as the sum of distances between all pairs of vertices in a tree. It was introduced as a structural descriptor for molecular graphs of alkanes, which are trees with vertex degrees of four at the most (chemical trees). The line graph L(G) of a graph G has the vertex set $V(L(\mathrm{G})) = E(\mathrm{G})$ and two distinct vertices of L(G) are adjacent if the corresponding edges of G have a common endvertex. It is known that the Wiener indices of a tree and of its line graph are always distinct. An infinite two-parameter family of growing chemical trees T with the property $W(\mathrm{T}) = W(L(L(\mathrm{T})))$ has been constructed.

INTRODUCTION

The Wiener index is a well-known topological index introduced as a structural descriptor for acyclic organic molecules.[1] It is defined as the sum of distances between all unordered pairs of vertices of a graph G:

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

where $d(u,v)$ is the number of edges in the shortest path connecting vertices u and v. This topological index is successfully used in QSAR and QSPR studies, including pharmacological and biological activity.[2–8] Mathematical properties of the Wiener index for some classes of chemical graphs can be found in recent reviews.[9,10]

The line graph, L(G), of a graph G has the vertex set $V(L(\mathrm{G})) = E(\mathrm{G})$ and two distinct vertices of the graph L(G) are adjacent if the corresponding edges of G have a common endvertex. The iterated line graph, $L^n(\mathrm{G})$, is defined as $L^n(\mathrm{G}) = L(L(\mathrm{G}^{n-1}))$, where $L^0(\mathrm{G}) = \mathrm{G}$. A graph $L^2(\mathrm{G})$ is called the quadratic line graph of G. The concept of line graph has found various applications in chemical research.[11,12] Invariants of iterated line graphs have been used for evaluating the branching and structural complexity of molecular graphs; for ordering isomeric structures and for designing novel topological indices.[13] An example of line graphs of a tree of order 9 is shown in Figure 1. For these graphs, $W(\mathrm{T}) = 108$, $W(L(\mathrm{T})) = 72$ and $W(L^2(\mathrm{T})) = 94$.

Buckley has demonstrated that the Wiener index of a tree and its line graph are always distinct.[14] Namely, if a tree T has n vertices, then $W(L(\mathrm{T})) = W(\mathrm{T}) - \binom{n}{2}$. In

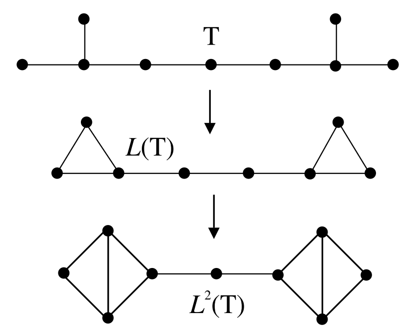

Figure 1. Tree T and its iterated line graphs.

* Authors to whom correspondence should be addressed. (E-mail: dobr@math.nsc.ru, omeln@math.nsc.ru)

this paper, we are interested in finding trees satisfying the following equality:

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

All trees of the order $n \leq 26$ with property (1) have been found by computing.[9,15,16] Several infinite families of such trees have been constructed as well.[16] We present a more general family of growing trees, which includes some of the previously known families.

Main Result

Consider a tree $\mathrm{T}_{k,s}$ (k, $s \geq 0$), shown in Figure 2. This tree is almost asymmetric (it has the unique two-element orbit of the automorphism group). Assume that its long left and right terminal paths have the length:

$$x_{k,s} = k(k-1)/2 + 6s^2 + 8s + 4 \quad \text{and}$$

$$y_{k,s} = k(k+3)/2 + 6s^2 + 12s + 7.$$

Therefore, trees $\mathrm{T}_{k,s}$ have $n = k^2 + k + 12s^2 + 28s + 19$ vertices and their diameter is equal to $diam(\mathrm{T}_{k,s}) = k^2 + k + 12s^2 + 28s + 15$. Every tree $\mathrm{T}_{k,s}$ is a so-called caterpillar in which the removal of all its endvertices results in a path. These trees are also chemical ones, *i.e.*, their vertex degrees are four at the most. It should be noted that all trees of the order $n \leq 18$ and $n = 20$ with property (1) are chemical trees.[16] The above described trees form an infinite family Υ:

$$\Upsilon = \cup_s \Upsilon_s = \cup_s \cup_k \mathrm{T}_{k,s}.$$

Element Υ_s of Υ is also an infinite set of trees.

Theorem. – For every integer $s \geq 0$, the family Υ_s generates an infinite set of trees $\mathrm{T}_{k,s}$ such that $\mathrm{T}_{k,s}$ satisfies equality (1) for every integer $k \geq 0$.

Two infinite families of trees constructed in Ref. 16 are members of Υ for $s = 0, 1$.

Formulas for the Wiener Index

The distance of a vertex v in a graph G, $d_{\mathrm{G}}(v)$, is the sum of distances between v and all other vertices of G, *i.e.*, $d_{\mathrm{G}}(v) = \Sigma_{u\in V(\mathrm{G})}\, d_{\mathrm{G}}(v,u)$. The Wiener index of the n-vertex path P_n is equal to $W(P_n) = n(n^2-1)/6$ and the distance of its endvertex v is equal to $d(v) = n(n-1)/2$. We use two well-known formulas to calculate the Wiener index for trees and their line graphs.

A vertex v is called the branching vertex of a tree if $\deg(v) \geq 3$. Denote by $B(\mathrm{T})$ the set of all branching vertices of an n-vertex tree T. Let $\mathrm{T}_1, \mathrm{T}_2, \ldots, \mathrm{T}_m$ be vertex disjoint subtrees of orders $p_1, p_2, \ldots, p_m$ attached to a branching vertex v (not all subtrees contain v). Then, the Wiener

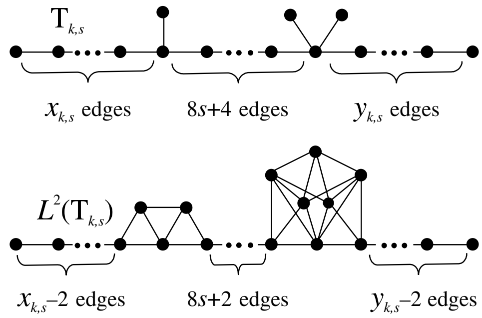

Figure 2. Tree $\mathrm{T}_{k,s}$ and its quadratic line graph.

index of T can be calculated by the Doyle-Graver formula:[17,18]

$$W(\mathrm{T}) = W(P_n) - \sum_{v\in B(\mathrm{T})} \sum_{1\leq i<j<k\leq m} p_i\, p_j\, p_k\,. \quad (2)$$

The Wiener index of a graph can be expressed through the Wiener index of its subgraphs under some graph operations.[9,19,20] Let a graph G be obtained from arbitrary graphs G_1 and G_2 of orders n_1 and n_2 by identifying vertices $v_1 \in V(\mathrm{G}_1)$ and $v_2 \in V(\mathrm{G}_2)$. Then

$$W(\mathrm{G}) = W(\mathrm{G}_1) + W(\mathrm{G}_2) + (n_1-1)d_{\mathrm{G}2}(v_2) + (n_2-1)d_{\mathrm{G}1}(v_1). \quad (3)$$

Formulas (2) and (3) will be used for trees and their line graphs, respectively.

Wiener Index for Trees of Υ_s

Let s be fixed. For every $k \geq 0$, the family Υ_s generates an infinite number of pairs of trees $\mathrm{T}_{k,s}$. Both trees of a pair have the same order, n. Consider the first tree (see Figure 2). Using the Doyle-Graver formula (2), we can write:

$$\begin{aligned}\mathrm{W}(\mathrm{T}_{k,s}) &= \mathrm{W}(P_n) - [x_{k,s}(y_{k,s} + 8s + 6) + (x_{k,s} + 8s + 5) + y_{k,s} + 2(x_{k,s} + 8s + 5)y_{k,s}] \\ &= [2k^6 + 6k^5 + (72s^2 + 168s + 111)k^4 + (144s^2 + 336s + 212)k^3 + \\ &\quad (864s^4 + 4032s^3 + 7296s^2 + 6048s + 1999)k^2 + \\ &\quad (864s^4 + 4032s^3 + 7224s^2 + 5928s + 1918)k + \\ &\quad 3456s^6 + 24192s^5 + 71568s^4 + 114464s^3 + \\ &\quad 105144s^2 + 52768s + 11352]/12.\end{aligned}$$

The quadratic line graph of $\mathrm{T}_{k,s}$ is depicted in Figure 2. It can be constructed from graph G_0 by consecu-

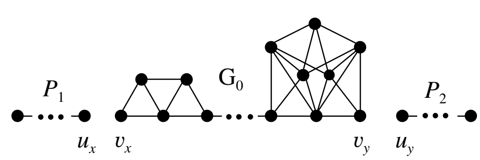

Figure 3. Graphs for constructing $L^2(\mathrm{T}_{k,s})$.

TABLE I. Parameters of the initial pairs of trees $T_{0,s}$ and $T^*_{0,s}$ of the family Υ_s

s	n	$x_{0,s}$	$y_{0,s}$	*diam*	W	s	n	$x_{0,s}$	$y_{0,s}$	*diam*	W
0	19	4	7	15	946	5	459	194	217	455	15961816
–	19	5	6	15	944	–	459	195	216	455	15961794
1	59	18	25	55	31912	6	619	268	295	615	39245802
–	59	19	24	55	31906	–	619	269	294	615	39245776
2	123	44	55	119	299466	7	803	354	385	799	85818216
–	123	45	54	119	299456	–	803	355	384	799	85818186
3	211	82	97	207	1533464	8	1011	452	487	1007	171466994
–	211	83	96	207	1533450	–	1011	453	486	1007	171466960
4	323	132	151	319	5540018	9	1243	562	601	1239	318931528
–	323	133	150	319	5540000	–	1243	563	600	1239	318931490

tively joining paths P_1 of length $x_{k,s} - 2$ and P_2 of length $y_{k,s} - 2$, as illustrated in Figure 3. Applying formula (3), we obtain $W(G_0) = (256s^3 + 1344s^2 + 1844s + 792)/3$. It is easy to see that $d_{G_0}(v_y) = 32s^2 + 68s + 40$. Let graph G_1 be obtained by identifying vertices v_y of G_0 and u_y of P_2. Then,

$$\begin{aligned} W(G_1) &= W(G_0) + W(P_2) + (n_{P2} - 1)d_{G_0}(v_y) + (n_{G_0} - 1)d(u_y) \\ &= (256s^3 + 1344s^2 + 1844s + 792)/3 + y_{k,s}(y^2_{k,s} - 1)/6 + (y_{k,s} - 2)(32s^2 + 68s + 40) + (8s + 13)(y_{k,s} - 1)(y_{k,s} - 2)/2 \\ &= [k^6 + 9k^5 + (36s^2 + 120s + 141)k^4 + (216s^2 + 720s + 711)k^3 + (432s^4 + 2880s^3 + 7860s^2 + 9240s + 4130)k^2 + (1296s^4 + 8640s^3 + 22608s^2 + 24480s + 9312)k + 1728s^6 + 17280s^5 + 74016s^4 + 161920s^3 + 196608s^2 + 126080s + 33312]/48. \end{aligned}$$

To construct the quadratic line graph $L^2(T_{k,s})$, one can identify vertices v_x of G_1 and u_x of P_1. By direct calculation, we obtain $d_{G_1}(v_x) = [k^4 + 6k^3 + (24s^2 + 80s + 55)k^2 + (72s^2 + 240s + 138)k + 144s^4 + 960s^3 + 2152s^2 + 2160s + 776]/8$. By (3), we have

$$\begin{aligned} W(L^2(T_{k,s})) &= W(G_1) + W(P_1) + (n_{P_1} - 1)d_{G_1}(v_x) + (n_{G_1} - 1)d(u_x) \\ &= W(G_1) + x_{k,s}(x^2_{k,s} - 1)/6 + (x_{k,s} - 2)d_{G_1}(v_x) + (8s + y_{k,s} + 10)(x_{k,s} - 1)(x_{k,s} - 2)/2 \\ &= [2k^6 + 6k^5 + (72s^2 + 168s + 111)k^4 + (144s^2 + 336s + 212)k^3 + (864s^4 + 4032s^3 + 7296s^2 + 6048s + 1999)k^2 + (864s^4 + 4032s^3 + 7224s^2 + 5928s + 1918)k + 3456s^6 + 24192s^5 + 71568s^4 + 114464s^3 + 105144s^2 + 52768s + 11352]/12. \end{aligned}$$

Comparing the Wiener indices, one can conclude that $W(T_{k,s}) = W(L^2(T_{k,s}))$.

The second tree $T^*_{k,s}$ of this pair has:

$$x^*_{k,s} = y_{k,s} - (4s + 2) \text{ and } y^*_{k,s} = x_{k,s} + (4s + 2),$$

where $x_{k,s}$ and $y_{k,s}$ are the corresponding quantities of the first tree $T_{k,s}$. By analogy with the previous calculations, one can obtain the following equalities:

$$W(T^*_{k,s}) = W(L^2(T^*_{k,s})) = W(T_{k,s}) - 2(4ks + 2k + 2s + 1).$$

Some numerical characteristics of trees $T_{0,s}$ and $T^*_{0,s}$ of the family Υ_s for the first values of s are presented in Table 1. Here, n and *diam* denote the order and the diameter of trees, respectively.

For manipulating cumbersome analytical expressions, the computer system for mathematics MAPLE® was used.

CONCLUSION

An infinite two-parameter family of growing chemical trees has been constructed. A tree of this family and its quadratic line graph have the same Wiener index. We believe that the following problem may be of interest for mathematical chemistry studies: characterizing molecular graphs by means of a topological index calculated for their derived structures. Since iterated line graphs reflect the branching of a tree, they serve as a good example of derived structures. We mention the simplest graph invariant, the number of edges of iterated line graphs, which has been applied for ordering molecular graphs and for related problems.[13] This is also a possible way of using a topological index that cannot be directly applied to initial structures. For example, consider trees and the Szeged index, *Sz*.[21] It is known that $Sz(G) = W(G)$ if and only if every block (maximal sub-graph without cut-vertices) of a graph G is a complete graph.[22] This implies that $Sz(T) = W(T)$ and $Sz(L(T)) = W(L(T))$ for any tree T. However, these indices may have distinct values for quadratic line graphs of trees. Therefore, we can associate with a tree T the value of the Szeged index of its quadratic line graph.

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SAŽETAK

Stabla, kvadratični linijski grafovi i Wienerov indeks

Andrey A. Dobrynin i Leonid S. Mel'nikov

Wienerov indeks *W* nekoga stabla je topologijski indeks koji predstavlja zbroj udaljenosti između svih čvorova u stablu. Uveden je kao strukturni indeks molekularnih grafova alkana (kemijskih stabala) u kojima valencija čvorova može poprimiti vrijednosti od 1 do najviše 4. Linijski graf $L(G)$ nekoga grafa G ima skup čvorova $V[L(G)]$ jednak broju bridova grafa G, a dva čvora $L(G)$ su povezana ako odgovarajući bridovi u G imaju zajednički čvor u kojem se susreću. Wienerov se indeks stabla i njegova linijskoga grafa razlikuju. Konstruirana je beskonačna dvoparametarska obitelj rastućih kemijskih stabala T sa svojstvom $W(T) = W(L(L(T)))$.