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WIENER INDEX, LINE GRAPHS AND THE CYCLOMATIC NUMBER*

Andrey A. Dobrynin and Leonid S. Mel'nikov

Sobolev Institute of Mathematics, Siberian Branch of the Russian Academy of Sciences, Novosibirsk 630090, Russia
E-mail: dobr@math.nsc.ru, omeln@math.nsc.ru

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Abstract

The Wiener index is a distance-based topological index defined as the sum of distances between all pairs of vertices in a graph. It is shown that for every $\lambda \geq 4$ there are planar bipartite graphs G with the cyclomatic number λ having the property $W(L(G)) = W(G)$, where $L(G)$ is the line graph of G.

1. Introduction

In this paper we are concerned with finite undirected connected graphs. The vertex and edge sets of G are denoted by $V(G)$ and $E(G)$, respectively. The cyclomatic number λ of a graph G is defined as $\lambda(G) = |E(G)| - |V(G)| + 1$. The line graph $L(G)$ of a graph G has vertices corresponding to the edges of G and two vertices are adjacent in $L(G)$ if their corresponding edges of G have a common endvertex. If u and v are vertices of G, then the number of edges in the shortest path connecting them is said to be their distance and is denoted by $d(u,v)$. The sum of distances from a vertex v to all vertices in a graph G is called the *distance* of this vertex, $d(v\,|\,G) = \sum_{u \in V(G)} d(u,v)$.

The Wiener index is a well-known distance-based topological index introduced as structural descriptor for acyclic organic molecules [26]. It is defined as the sum of distances between all unordered pairs of vertices of a simple graph G:

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v) = \frac{1}{2} \sum_{v \in V(G)} d(v\,|\,G).$$

*This paper is dedicated to Professor O. E. Polansky in recognition of his valuable contribution to the Chemical Graph Theory.

Mathematical properties and chemical applications of the Wiener index have been intensively studied in the last thirty five years. Nowadays, the Wiener index is one of the best understood and most frequently used molecular shape descriptors. It found numerous applications in the modelling of physico-chemical, pharmacological and biological properties of organic molecules. The bibliography on the Wiener index and its applications can be found in books [5, 16, 24, 25] and reviews [4, 6, 7, 9, 18, 19, 20, 23]).

One of the interesting approaches in mathematical chemistry studies is to characterize molecular graphs by means of parameters calculated for their derived structures. Since line graphs reflect branchings of initial graphs, they serve as a good example of derived structures. Invariants of line graphs have been applied for the evaluation of structural complexity of molecular graphs, for ordering of structures and for design of novel topological indices [1, 2, 11, 13, 17].

In this paper, we are interesting in finding of graphs satisfying the following equality

$$W(L(G)) = W(G) \tag{1}$$

and having prescribe cyclomatic numbers $\lambda(G)$. It was shown that the Wiener index of a tree ($\lambda(G) = 0$) and its line graph are always distinct [3]. It is a well-known fact that n-vertex graph G is isomorphic to $L(G)$ if and only if G is the simple cycle C_n. Therefore, the equality (1) holds for simple cycles in a trivial manner. For all other unicyclic graphs, $W(L(G)) < W(G)$ [12]. Therefore, if a cycle-containing graph, except a simple cycle, satisfies the equality (1), then it has at least two cycles ($\lambda(G) = 2$) [12, 15]. There are exactly 26 minimal bicyclic graphs of order 9 having property (1) [8, 14]. The numbers of bicyclic graphs of order 10, 11 and 12 satisfying equality (1) are 166, 503 and 1082, respectively [8]. Series of bicyclic graphs with increasing order have been constructed in [15]. Minimal tricyclic graphs ($\lambda(G) = 3$) with property (1) have 12 vertices (71 graphs) [8]. Some evaluations of the difference between the Wiener index of a graph and its line graph in terms of the number of vertices and edges are presented in [12]. The following question was put forward in [8]:

Do there exist graphs G with cyclomatic number $\lambda = \lambda(G)$ having property (1) for every $\lambda \geq 4$?

Two infinite families of such nonbipartite graphs with increasing cyclomatic number are constructed in [10]. However, the obtained λ does not cover all possible values of the

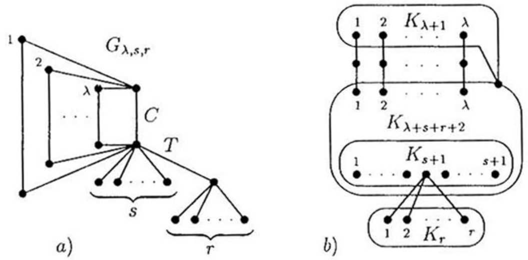

Figure 1. Graph $G_{\lambda,s,r}$ and its line graph.

cyclomatic number and the difference between neighbors values of λ rapidly increases. In this paper, we give a complete answer to this question by constructing two infinite families of graphs with corresponding properties. Moreover, we show that the difference $W(L(G)) - W(G)$ may be equal to an arbitrary integer.

2. Main results

Consider the graph $G_{\lambda,s,r}$ shown in Figure 1a. By construction, it has cyclomatic number λ and order $2\lambda + s + r + 3$. Obviously, $G_{\lambda,s,r}$ is a planar bipartite graph for every λ, s and r. The structure of the line graph $L(G_{\lambda,s,r})$ is depicted in Figure 1b. Its complete subgraphs are drawn without edges. Let $\Delta W(G) = W(L(G)) - W(G)$.

Proposition 1. *For every $\lambda \geq 2$, there are planar bipartite graphs G with the cyclomatic number λ such that $\Delta W(G) = 0$.*

Proof. The graph $G_{\lambda,s,r}$ can be obtained by identifying vertex u of the cyclyc graph C and vertex v of the tree T (see Figure 1). In order to calculate the Wiener index of $G_{\lambda,s,r}$, it is convenient to use the following formula [21, 22]:

$$W(G) = W(C) + W(T) + (n_T - 1)d(u\,|\,C) + (n_C - 1)d(v\,|\,T).$$

where n_G denotes the number of vertices in a graph G. Since $W(C) = 5\lambda^2 + 2\lambda + 1$, $W(T) = s^2 + r^2 + 3sr + 2s + 2r + 1$ and $d_C(u) = 3\lambda + 1$, $d_T(v) = s + 2r + 1$, we have

$$W(G_{\lambda,s,r}) = 5\lambda^2 + 7\lambda + 5\lambda s + 7\lambda r + s^2 + r^2 + 3sr + 4s + 5r + 4.$$

Table 1: Families of graphs induced by $G_{\lambda,2\lambda-4,\lambda+1}$ (top part) and $G_{\lambda,2\lambda-6,\lambda+4}$.

λ	2	3	4	5	6	7	8	9	10	11	12
n	10	15	20	25	30	35	40	45	50	55	60
(s,r)	(0,3)	(2,4)	(4,5)	(6,6)	(8,7)	(10,8)	(12,9)	(14,10)	(16,11)	(18,12)	(20,13)
W	104	256	474	758	1108	1524	2006	2554	3168	3848	4594
n	-	16	21	26	31	36	41	46	51	56	61
(s,r)	-	(0,7)	(2,8)	(4,9)	(6,10)	(8,11)	(10,12)	(12,13)	(14,14)	(16,15)	(18,16)
W	-	301	540	845	1216	1653	2156	2725	3360	4061	4828

The line graph consists of complete subgraphs and has diameter 3. Therefore, its Wiener index can be easily calculated. Namely,

$$W(L(G_{\lambda,s,r})) = (17\lambda^2 + 9\lambda + 10\lambda s + 16\lambda r + s^2 + r^2 + 4sr + 3s + 5r + 2)/2.$$

We construct desired graphs by specifying parameters s and r in $G_{\lambda,s,r}$. It is a natural idea to represent these parameters as functions in λ. Let $s = 2\lambda-4$, $r = \lambda+1$ or $s = 2\lambda-6$, $r = \lambda + 4$. The corresponding graphs $G_{\lambda,2\lambda-4,\lambda+1}$ and $G_{\lambda,2\lambda-6,\lambda+4}$ induce two infinite families when λ tends to infinity. These graphs have order 5λ and $5\lambda + 1$, respectively. Their Wiener indices are equal to $W(G_{\lambda,2\lambda-4,\lambda+1}) = W(L(G_{\lambda,2\lambda-4,\lambda+1})) = 33\lambda^2 - 13\lambda - 2$ for all $\lambda \geq 2$ and $W(G_{\lambda,2\lambda-6,\lambda+4}) = W(L(G_{\lambda,2\lambda-6,\lambda+4})) = 33\lambda^2 + 8\lambda - 20$ for all $\lambda \geq 3$. $\square$

Parameters of the constructed graphs for small cyclomatic numbers are presented in Table 1. Specifying s and r, we can formulate more general result concerning possible values of $\Delta W(G)$.

Proposition 2. *For every integer $t \geq 0$, there are planar bipartite graphs G and H such that $\Delta W(G) = t$ and $\Delta W(H) = -t$.*

Proof. To prove Proposition 2, it is sufficient to examine graphs $G_{\lambda,2\lambda-5,\lambda+2}$ and $G_{\lambda,2\lambda-3,\lambda}$. For the difference of the Wiener indices of $G_{\lambda,s,r}$ and $L(G_{\lambda,s,r})$, we can write

$$\Delta W(G_{\lambda,s,r}) = (7\lambda^2 - 5\lambda + 2\lambda r - s^2 - r^2 - 2sr - 5s - 5r - 6)/2.$$

Then $\Delta W(G_{\lambda,2\lambda-5,\lambda+2}) = \lambda$ for $\lambda \geq 3$ and $\Delta W(G_{\lambda,2\lambda-3,\lambda}) = -\lambda$ for $\lambda \geq 2$.

The constructed graphs don't cover values $\Delta W \in \{-1, 1, 2\}$. Consider planar bipartite graphs shown in Figure 2. We have $\Delta W(G_1) = 85 - 86 = -1$, $\Delta W(G_2) = 60 - 59 = 1$ and $\Delta W(G_3) = 84 - 82 = 2$. $\square$

In conclusion we note that the obtained graphs have three vertices of large degree. We believe that the following problem may be of interest for researchers in mathematical

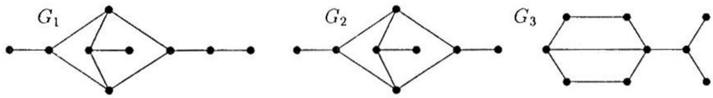

Figure 2. Graphs G with $\Delta W(G) \in \{-1, 1, 2\}$.

chemistry: to construct an infinite family of growing chemical graphs G (i.e. graphs with vertex degrees at most four) with arbitrary cyclomatic number satisfying equality $\Delta W(G) = 0$.

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