

On Peripheral Wiener Index: Line Graphs, Zagreb Index, and Cut Method

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(Received December 24, 2018)

Abstract

The peripheral Wiener index, $PW(G)$ is the sum of the distances of all pairs of vertices in the periphery of a graph G . In this paper it is shown that, an arbitrary graph G is an induced subgraph of a graph H for which $PW(H) = PW(L(H))$ holds, where $L(K)$ is the line graph of K . Using Pell-like equations, infinite families of graphs G are constructed for which $PW(G) = PW(L(G))$ holds. A connection between the peripheral Wiener index and the Zagreb index for graphs of small diameter is presented. It is also demonstrated that the partition distance approach applicable to the peripheral Wiener index, making some earlier results as very special cases of this approach.

1 Introduction

Because of the seminal Wiener's discovery of a close relation between boiling points of certain alkanes and the Wiener index [32], it became perceptible that graph invariants, also addressed to as topological indices, can be used to predict properties of chemical

compounds. During the related history, many additional topological indices have been studied, in particular several Wiener-like indices such as the hyper-Wiener index [21], the reciprocal Wiener index [16], and the terminal Wiener index [11, 27], to name just a few of them.

Unless stated otherwise, the graphs considered in this paper are finite and connected. If G is a graph, then $m(G)$ denotes the size of G and $n(G)$ the order of G . Let $d_G(u, v)$ denote the usual shortest path distance between vertices u and v in G . The *eccentricity* $e_G(v)$ or $e(v)$ of a vertex v is the distance to a furthest vertex from v in G . The *diameter*, $\text{diam}(G)$ of G is the maximum eccentricity of G . A vertex v with $e_G(v) = \text{diam}(G)$ is called a *peripheral vertex* of G . The set of peripheral vertices of G is called the *periphery* of G and denoted by $P(G)$. We will also use the notation $p(G) = |P(G)|$ for the order of the periphery. We note in passing that the periphery of a graph has many applications (see eg. [19, 20]), in particular because (as stated in [4]), the peripheral attachments of a molecule are quite often the deciding factor in chemical reactions; cf. also [33].

In [24] another Wiener-like topological index was introduced as follows. If G is a graph, then its *peripheral Wiener index* $PW(G)$ is the sum of the distances between all pairs of peripheral vertices of G , that is,

$$PW(G) = \sum_{\{u,v\} \subseteq P(G)} d(u, v).$$

The peripheral Wiener index received an immediate attention. In [5] the main focus is on the peripheral Wiener index of trees, while in [15] different upper and lower bounds are proved. Moreover, sharp bounds on the difference between the Wiener index and the peripheral Wiener index are derived. In this paper we continue the study of the peripheral Wiener index with two main goals: to understand its behaviour on line graphs and to demonstrate how the cut method is applicable to the peripheral Wiener index.

Recall that the *line graph* $L(G)$ of a graph G is the graph with $V(L(G)) = E(G)$, two vertices of $L(G)$ being adjacent if and only if the corresponding edges of G are adjacent. The concept of line graph has found various applications in chemical research, cf. [6, 10, 12, 25]. In particular, iterated line graphs turned out to be chemically important, see [7, 13, 30]. In this paper we are interested in cycle containing graphs G with the property

$$PW(G) = PW(L(G)). \tag{1}$$

The related problem has been extensively studied for the Wiener index, a survey of these developments is given in [23].

Constructions of unicyclic and bicyclic graphs for which one of $PW(G) > PW(L(G))$, $PW(G) < PW(L(G))$, or $PW(G) = PW(L(G))$ holds can be seen in [29]. In Section 2 we show that any graph G is an induced subgraph of a graph H , such that $PW(H) = PW(L(H))$ holds. In Section 3 we give two infinite families of graphs G for which $PW(G) = PW(L(G))$ hold. Pell-like Diophantine equations are essential for their analysis. Then, in Section 4, we give a connection between the peripheral Wiener index and the Zagreb index for graphs of small diameter. In Section 5 we point out that the very general partition distance approach from [18] is applicable to the peripheral Wiener index, making several earlier results a very special cases of this approach. A couple of future research directions are indicated at the end.

2 Embedding graphs into graphs for which (1) holds

In this section we prove the following:

Theorem 2.1. *If G is a graph, then there exists a graph H such that G is an induced subgraph of H and $PW(H) = PW(L(H))$. Moreover, $H - V(G)$ is a bicyclic graph.*

Proof. Let $H_{p,q}$, $p, q, \geq 2$, be the graph obtained from disjoint cycles C_{2p+1} and C_{2q} by identifying a vertex of C_{2p+1} with a vertex of C_{2q} . Setting $V(C_{2p+1}) = \{u_0, u_1, \dots, u_{2p}\}$ and $V(C_{2q}) = \{w_0, w_1, \dots, w_{2q-1}\}$, we may assume without loss of generality that in $H_{p,q}$ the vertex u_0 is identified with w_0 , see Fig. 1.

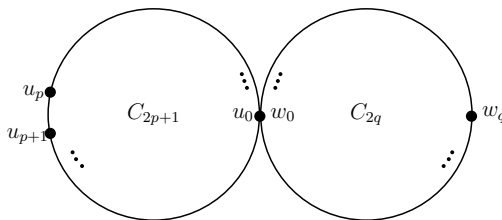


Figure 1. Graph $H_{p,q}$.

Let now H be the graph obtained from the disjoint union of G and $H_{p,q}$ by adding all possible edges between the vertices of G and the vertices $u_0 = w_0$, u_{2p} , and w_{2q-1} . In

other words, in H there is a join between G and the subgraph of $H_{p,q}$ induced by the vertices $u_0 = w_0, u_{2p}$, and w_{2q-1} . See Fig. 2 where H is shown (left) and $L(H)$ (right).

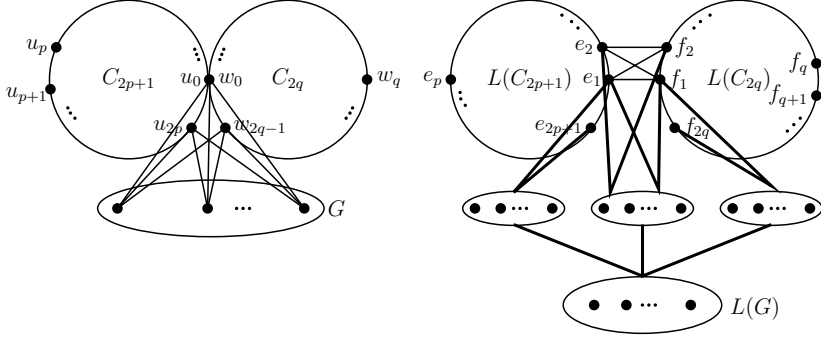


Figure 2. Graphs H (left) and $L(H)$ (right)

It is now straightforward to verify that $P(H) = \{u_p, u_{p+1}, w_q\}$ and consequently $PW(H) = 2(p + q) + 1$. Similarly, using the notation for the vertices of $L(H)$ as shown in Fig. 2, it is also a routine to check that $P(L(H)) = \{e_p, f_q, f_{q+1}\}$. But then $PW(L(H)) = 2(p + q) + 1$ and hence $PW(H) = PW(L(H))$. Since, clearly, G is an induced subgraph of H and $H - V(G) = H_{p,q}$ is a bicyclic graph, we are done. ■

Selecting G to be the empty graph in Theorem 2.1, we infer that the graphs $H_{p,q}$ (as defined in the proof of the theorem) form an infinite family of bicyclic graphs for which (1) holds.

3 Two infinite families and Pell-like equations

In this section we propose two families of graphs that lead to infinite families of graphs with an arbitrary cyclomatic number that fulfil (1). Since a cycle of a graph induces a cycle of same length in its line graph, the increase of the order of $L(G)$ should be compensated by decreasing the distances between vertices in $L(G)$.

The first family consists of the graphs $G(r, s, \mu)$ as presented on the left part of Fig. 3, where the below part of the figure displays $L(G(r, s, \mu))$. The notation μ for the number $\mu - 1$ of triangles above the edge v_1v_2 is selected because $\mu(G(r, s, \mu)) = \mu$, where $\mu(X)$ is the *cyclomatic number* of X defined as $\mu(X) = m(X) - n(X) + 1$.

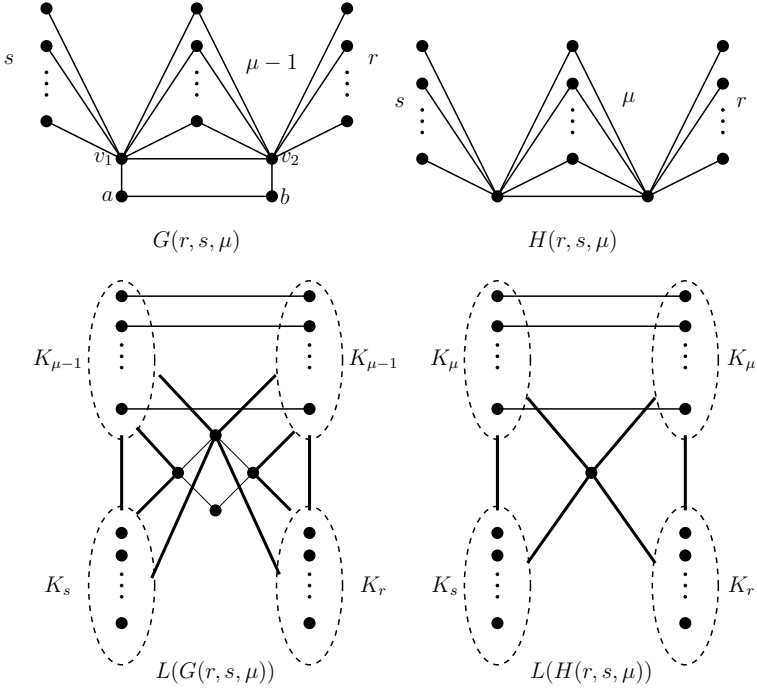


Figure 3. Graphs $G(r, s, \mu)$, $H(r, s, \mu)$, and their line graphs.

To simplify the notation, set $G = G(r, s, \mu)$. Note that the order of G is $\mu + s + r + 3$ and that $p(G) = s + r + 2$. Moreover, the order of $L(G)$ is $2\mu + s + r + 2$ and $L(G)$ is a self-centered graph, that is, every vertex of it lies in the periphery. Hence

$$\begin{aligned} PW(G) &= s^2 + r^2 + 3sr + 4r + 4s + 1, \\ PW(L(G)) &= \frac{1}{2} (6s\mu + 6r\mu + 4sr + s^2 + r^2 + 5s + 5r + 6\mu^2 + 8\mu + 2). \end{aligned}$$

If the equality holds in (1) for G , then we get the following quadratic equation with respect to the parameters s, r and μ :

$$s^2 + (2r - 6\mu + 3)s + (-6\mu^2 - 6\mu r - 8\mu + r^2 + 3r) = 0.$$

A suitable root of this equation is equal to

$$s = \frac{(6\mu - 2r - 3) + \sqrt{60\mu^2 - 4\mu + 9}}{2}. \quad (2)$$

The number s is an integer if and only if the radicand in (2) is an odd perfect square, that is, $y^2 = 60\mu^2 - 4\mu + 9$ for some odd integer y . Applying substitution $x = 30\mu - 1$, equality (2) can be rewritten as:

$$s + r = \frac{x + 5y}{10} - \frac{7}{5}, \quad (3)$$

with the relation

$$15y^2 - x^2 = 134, \quad (4)$$

which is a Pell-like Diophantine equation, see [28]. It has an infinite number of solutions. All solutions of equation (4) can be generated by the following explicit formulae for integers $n \geq 1$:

$$\begin{cases} x_n &= 4x_{n-1} + 15y_{n-1} \\ y_n &= x_{n-1} + 4y_{n-1} \end{cases} \quad (5)$$

with the initial values $x_0 + y_0\sqrt{15} = 1 + 3\sqrt{15}$ or $x_0 + y_0\sqrt{15} = 41 + 11\sqrt{15}$, since both initial values are fundamental solutions of (4).

Consider next graphs $H(r, s, \mu)$ and $L(H(r, s, \mu))$ as shown in Fig. 3. We again use the parameter μ to indicate that the cyclomatic number of $H(r, s, \mu)$ is μ .

To simplify the presentation, set for the rest $H = H(r, s, \mu)$. The graph H has $\mu + s + r + 2$ vertices among which $s + r$ are peripheral. So we have

$$\begin{aligned} PW(H) &= 3sr + s^2 + r^2 - s - r. \\ PW(L(H)) &= \frac{1}{2}(6\mu s + 6\mu r + 4rs + s^2 + r^2 - s - r + 6\mu^2 - 4\mu). \end{aligned}$$

If the equality holds in (1) for H , then

$$s^2 + 3sr - s + r^2 - r = \frac{1}{2}(6\mu s + 6\mu r + 4rs + s^2 + r^2 - s - r + 6\mu^2 - 4\mu).$$

Solving this for s , we have a suitable solution of the form

$$s = \frac{6\mu - 2r + 1 + \sqrt{60\mu^2 - 4\mu + 1}}{2}. \quad (6)$$

The number s is an integer if and only if $y^2 = 60\mu^2 - 4\mu + 1$, for some odd integer y . Using substitution $x = 30\mu - 1$, equality (6) can be presented as:

$$s + r = \frac{x + 5y}{10} + \frac{3}{5}, \quad (7)$$

with the relation

$$15y^2 - x^2 = 14, \quad (8)$$

which is a Pell-like Diophantine equation.

Solution of (8) can be obtained from the explicit equations for odd n

$$\begin{cases} x_n &= 4x_{n-1} + 15y_{n-1} \\ y_n &= x_{n-1} + 4y_{n-1} \end{cases} \quad (9)$$

with the initial condition $x_0 + y_0\sqrt{15} = 1 + \sqrt{15}$ or $x_0 + y_0\sqrt{15} = 11 + 3\sqrt{15}$, since both initial values are fundamental solutions of (9) .

The solutions of (4) and (8) have basically the same form, except their initial conditions. The first solutions are presented in Table 1. Here the value of N in the Diophantine equations $15y^2 - x^2 = N$ in (4) and (8) are shown. Below the value $N = 134$ the first two columns are for the first initial condition $x_0 + y_0\sqrt{15} = 1 + 3\sqrt{15}$ and the next two columns are for the second initial condition $x_0 + y_0\sqrt{15} = 41 + 11\sqrt{15}$. Similarly, below the value $N = 14$ the first two column are for the first initial condition $x_0 + y_0\sqrt{15} = 1 + \sqrt{15}$ and the next two columns are for the second initial condition $x_0 + y_0\sqrt{15} = 11 + 3\sqrt{15}$.

Table 1. First solutions for recurrence relations (5) and (9)

	$N = 134$				$N = 14$			
n	x_n	y_n	x_n	y_n	x_n	y_n	x_n	y_n
0	1	3	41	11	1	1	11	3
1	49	13	329	85	19	5	89	23
2	391	101	2591	669	151	39	701	181
3	3079	795	20399	5267	1189	307	5519	1425
4	24241	6259	160601	41467	9361	2417	43451	11219
5	190849	49277	1264409	326469	73699	19029	342089	88327
6	1502551	387957	9954671	2570285	580231	149815	2693261	695397
7	11829559	3054379	78372959	20235811	4568149	1179491	21203999	5474849

To construct an infinite sequence of graphs with increasing cyclomatic number that satisfy (1), we find an infinite sequence of solutions of (4) and (8) with integer μ .

Consider the family based on the graph G . Since $\mu = \frac{x+1}{30}$, the values of x must equal to $29 \pmod{30}$ so that μ will has integer value. These values of x depend on the initial values $x_0 + y_0\sqrt{15}$. For the initial value $1 + 3\sqrt{15}$, One can easily observe that the values of x are either $1 \pmod{30}$ or $19 \pmod{30}$, which are irrelevant.

For the initial value $41 + 11\sqrt{15}$, the values of x are either $11 \pmod{30}$ or $29 \pmod{30}$. Thus μ has integer values for an odd integer n for which the initial value $41 + 11\sqrt{15}$ is taken. Few examples of respective values of x_n and y_n are presented in Table 2 for which μ has integer values.

Table 2. First five solutions of recurrence relation (5) for which μ has integer values.

n	x_n	y_n	μ
1	329	85	11
3	20399	5267	680
5	1264409	236469	42147
7	78372959	20235811	2612432
9	4857859049	1254293813	161928635

Since $s + r = 3\mu + \frac{y-3}{2}$, there are at least $\lfloor \frac{6\mu+y-3}{4} \rfloor + 1$ non-isomorphic graphs having property (1) for a given μ .

Consider now the family based on the graph H . In similar way as in the case for graph G , since $\mu = \frac{x+1}{30}$, the values of x must equal to 29 (mod 30) so that μ has integer values. The values of x_n , for odd integer n satisfy this condition with initial value $x_0 + y_0\sqrt{15} = 11 + 3\sqrt{15}$. The first five values of x_n and y_n are presented in Table 3 for which μ has integer values.

Table 3. First five solutions of recurrence relation (9) for which μ has integer values.

n	x_n	y_n	μ
1	83	233	3
3	5519	1425	184
5	342089	88327	11403
7	21203999	43103395	706800
9	1314305849	339352311	43810195

Since $s + r = 3\mu + \frac{y+1}{2}$, there are at least $\lfloor \frac{6\mu+y+1}{4} \rfloor + 1$ non-isomorphic graphs having property (1) for given μ .

4 On $PW(L(G))$ and the first Zagreb index

In this short section we give a connection between the peripheral Wiener index of line graphs of small diameter and the first Zagreb index. The latter index of a graph G is defined as

$$M_1(G) = \sum_{v \in V(G)} \deg(v)^2,$$

and is one of the oldest and most thoroughly studied topological indices. It was introduced in 1972 by Gutman and Trinajstić [14], surveyed 30 years after in [8], while 45 years after

the bounds for the Zagreb indices were surveyed in [3]. The first Zagreb index keeps going to be in the focus of researchers, cf. [1, 2, 26]. The connection reads as follows.

Theorem 4.1. *If G is a graph with $\text{diam}(L(G)) = 2$, then*

$$PW(L(G)) = \binom{m(G) + 1}{2} + \binom{p(L(G))}{2} - \frac{1}{2}M_1(G).$$

Proof. Clearly, $n(L(G)) = m(G)$, while the number of edges of $L(G)$ can be expressed as follows:

$$\begin{aligned} m(L(G)) &= \sum_{v \in V(G)} \binom{\deg(v)}{2} = \frac{1}{2} \sum_{v \in V(G)} \deg(v)^2 - \frac{1}{2} \sum_{v \in V(G)} \deg(v) \\ &= \frac{1}{2}M_1(G) - m(G). \end{aligned}$$

Since $\text{diam}(L(G)) = 2$, the following relation follows from [24, Theorem 2]:

$$PW(L(G)) = \binom{n(L(G))}{2} + \binom{p(L(G))}{2} - m(L(G)).$$

Consequently,

$$\begin{aligned} PW(L(G)) &= \binom{m(G)}{2} + \binom{p(L(G))}{2} - \left(\frac{1}{2}M_1(G) - m(G)\right) \\ &= \binom{m(G) + 1}{2} + \binom{p(L(G))}{2} - \frac{1}{2}M_1(G). \end{aligned}$$

■

For regular graphs Theorem 4.1 simplifies as follows. The computation is straightforward and hence omitted.

Corollary 4.2. *If G is an r -regular graph with $\text{diam}(L(G)) = 2$, then*

$$PW(L(G)) = \frac{n(G)r(n(G)r - 4r + 2)}{8} + \binom{p(L(G))}{2}.$$

5 Peripheral Wiener index and cut method

In this section we relate the peripheral Wiener index with the cut method. More precisely, we demonstrate that the very general approach from [18] applies to the peripheral Wiener index which in turn implies that some earlier stated results appear as very special cases.

Let G be a graph and let $\mathcal{P} = \{V_1, \dots, V_k\}$ be a partition of $V(G)$. Let $f_{\mathcal{P}} : V(G) \rightarrow [k] = \{1, \dots, k\}$ be the index function of $\mathcal{P}$ defined with $f_{\mathcal{P}}(v) = i$, where $v \in V_i$. The *partition distance* $W_{\mathcal{P}}(G)$ of G with respect to $\mathcal{P}$ is defined as:

$$W_{\mathcal{P}}(G) = \sum_{\substack{\{u,v\} \\ f_{\mathcal{P}}(u) = f_{\mathcal{P}}(v)}} d_G(u, v).$$

That is, in $W_{\mathcal{P}}(G)$ only the distance between those pairs of vertices are counted which lie in the same part of the partition $\mathcal{P}$.

Now, let G be a graph with the periphery $P(G)$ and let $V(G) - P(G) = \{v_1, \dots, v_k\}$. Let us call the partition $\mathcal{T} = \{P(G), \{v_1\}, \dots, \{v_k\}\}$ of $V(G)$ the *peripheral partition*. Thus, if $\mathcal{T}$ is the peripheral partition of $V(G)$, then we have:

$$PW(G) = W_{\mathcal{T}}(G).$$

One of the main theorems from [18] then, for the case of the peripheral Wiener index, reduces to the following result.

Theorem 5.1. *Let G be a connected graph and $\{F_1, \dots, F_r\}$ the Θ^* -partition of $E(G)$. Then*

$$PW(G) = \sum_{i=1}^r W(G/F_i, w_i),$$

where $w_i(C) = |C \cap P(G)|$ for any $C \in V(G/F_i)$.

We do not formally define here the concepts used in Theorem 5.1, the reader can find them in [18] or in [17], where a survey on the cut method is given. The method itself has a long history, see [31] (references therein) for a recent nice development.

Let us conclude with a remark that the following result from [24, Theorem 5] is a very special case of Theorem 5.1. If T is a tree and $e \in E(T)$, then let $p_1(e)$ and $p_2(e)$ be the number of peripheral vertices of T lying on the two sides of e , respectively. Then:

Proposition 5.2. *If T is a tree, then*

$$PW(T) = \sum_{e \in E(T)} p_1(e) \cdot p_2(e).$$

6 Concluding remarks

In this paper we were in particular interested in graphs G for which $PW(G) = PW(L(G))$ holds. A more general (and also interesting) question is to find, or, ideally, characterize

the graphs G for which

$$PW(G) = PW(L^k(G))$$

holds, where k is a fixed, positive integer. The related problem for the Wiener index was formulated in [9]. See also [22], where the equation $W(L^3(T)) = W(T)$ is solved for trees, and references therein.

At the end of Section 2 we have observed that the graphs $H_{p,q}$ are bicyclic graphs for which (1) holds. It would be of interest to consider the problem of the existence of bicyclic graphs G for which $PW(G) = PW(L^k(G))$ holds for some fixed integer $k \geq 2$.

Acknowledgments: We are grateful to a referee for a careful reading of our manuscript, in particular for pointing out a couple of miscalculations.

Sandi Klavžar acknowledges the financial support from the Slovenian Research Agency (research core funding No. P1-0297 and project Contemporary invariants in graphs No. J1-9109). Afework T. Kahsay acknowledges the financial support from the Ministry of Education of the Federal Democratic Republic of Ethiopia.

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