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A Note on the Maximum Value of $W(L(G))/W(G)$

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Abstract

The line graph $L(G)$ of a graph G is defined as a graph having vertex set identical with the set of edges of G and two vertices of $L(G)$ are adjacent if and only if the corresponding edges are incident in G. Higher iteration $L^i(G)$ is obtained by repeatedly applying the line graph operation i times. Wiener index $W(G)$ of a graph G is defined as the sum of distances which runs over all pairs of vertices in G. The problem of establishing the extremal values and extremal graphs for the ratio $W(L^i(G))/W(G)$ was proposed by Dobrynin and Melnikov [Mathematical Chemistry Monographs, Vol. 12, 2012, pp. 85-121]. In this paper we establish the maximum value and characterize the extremal graphs for $i = 1$. In doing so, we derive unexpectedly an interesting relation that involves the Gutman index and the first Zagreb index.

1 Introduction

Let G be a graph with $n = |V(G)|$ vertices and $m = |E(G)|$ edges. In this paper we assume G is simple and connected, unless explicitly stated otherwise. The degree of a vertex $u \in V(G)$ is denoted by $d(u)$. For any two vertices $u, v \in V(G)$ the distance between u and v is denoted by $d(u, v)$. The Wiener index of the graph G is defined by

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

and it is introduced in [16] as a quantity that correlates well with chemical properties of molecules represented by the graphs. Wiener index attracted lot of interest and has become one of the most extensively studied topological indices (see [12,18]). One direction of research is the relation of Wiener index of a graph and the corresponding line graph.

The line graph $L(G)$ of a graph G is defined as a graph having vertex set identical with the set of edges of G and two vertices of $L(G)$ are adjacent if and only if the corresponding edges are incident in G. Higher iterations of the line graph are defined by

$$L^i(G) = \begin{cases} G & \text{for } i = 0, \\ L(L^{i-1}(G)) & \text{for } i > 0. \end{cases}$$

Amongst many interesting papers on Wiener index of line graphs we cite [1,10,11,17]. A problem of establishing the extremal values and graphs for the ratio $W(L^i(G))/W(G)$ for $i \geq 1$ was proposed in [2]. The minimal value of the ratio for $i = 1$ and the corresponding minimal graphs are established in [11]. In this paper we will establish the maximal value for $i = 1$ and characterize all maximal graphs. The problem remains open for $i > 1$.

In order to establish the main result of the paper we will derive the upper bound on $W(L(G))$ in terms of the Gutman and the first Zagreb index of a graph G, so let us introduce those two topological indices. The Gutman index $\mathrm{Gut}(G)$ and the first Zagreb index $M_1(G)$ of a graph G are defined by

$$\mathrm{Gut}(G) = \sum_{\{u,v\} \subseteq V(G)} d(u)d(v)d(u,v) \quad \text{and} \quad M_1(G) = \sum_{u \in V(G)} d^2(u).$$

The first Zagreb index was introduced in [7], and has attracted a lot of interest since [3, 6, 8, 13, 14]. Gutman index was first introduced in [5], for recent papers involving Gutman index and similar degre-distance based indices see [4, 15].

2 Main results

For two edges $e = uv$ and $f = xy$ from a graph G we define

$$D(e, f) = \frac{1}{4}(d(u, x) + d(u, y) + d(v, x) + d(v, y)).$$

If a pair of edges $e = uv$ and $f = xy$ share an end-vertex, say $v = x$, then obviously

$$D(e, f) = \begin{cases} 1 & \text{if } uy \notin E(G), \\ \frac{3}{4} & \text{if } uy \in E(G). \end{cases} \tag{1}$$

We now wish to express $d_{L(G)}(e, f)$ in terms of $D(e, f)$. First, notice that for every $\{e, f\} \subseteq E(G)$ it holds that

$$d_{L(G)}(e, f) = \min\{d(u, x), d(u, y), d(v, x), d(v, y)\} + 1 \leq D(e, f) + 1. \tag{2}$$

In the case when a pair of edges e and f from G share an end-vertex, we can obtain even tighter bound from (1), as in that case we have

$$d_{L(G)}(e,f) = 1 \leq D(e,f) + 1 - \frac{3}{4}. \tag{3}$$

Now, we first derive the upper bound on $W(L(G))$ in terms of Gut(G) and $M_1(G)$ in the following lemma.

Theorem 1 *For a graph G with n vertices and m edges it holds that*

$$W(L(G)) \leq \frac{1}{4}\mathrm{Gut}(G) - \frac{3}{8}M_1(G) + \frac{1}{2}m^2$$

with equality if and only if $G = K_n$.

Proof. By the definition of Wiener index we have

$$W(L(G)) = \sum_{\{e,f\}\subseteq E(G)} d_{L(G)}(e,f).$$

Using upper bounds on $d_{L(G)}(e,f)$ from (2) and (3) we further obtain

$$\begin{aligned} W(L(G)) &\leq \sum_{\{e,f\}\subseteq E(G)} (D(e,f)+1) - \frac{3}{4}\sum_{u\in V(G)} \binom{d(u)}{2} \\ &= \sum_{\{e,f\}\subseteq E(G)} D(e,f) + \binom{m}{2} - \frac{3}{4}\sum_{u\in V(G)} \frac{d(u)(d(u)-1)}{2}. \end{aligned}$$

By the definition of $D(e,f)$ we have

$$\sum_{\{e,f\}\subseteq E(G)} D(e,f) = \frac{1}{4}\sum_{\{e,f\}\subseteq E(G)} (d(u,x)+d(u,y)+d(v,x)+d(v,y)). \tag{4}$$

Notice that for a pair of vertices $\{u,v\} \subseteq V(G)$ which are not adjacent, the distance $d(u,v)$ will appear in the sum (4) precisely $d(u)d(v)$ times, i.e. for as many pairs of edges. On the other hand, if u and v are adjacent, then the distance $d(u,v)$ will appear in the sum $d(u)d(v) - 1$ times. So, we conclude

$$\begin{aligned} \sum_{\{e,f\}\subseteq E(G)} D(e,f) &= \frac{1}{4}\sum_{\substack{\{u,v\}\subseteq V(G)\\ uv\notin E(G)}} d(u)d(v)d(u,v) + \frac{1}{4}\sum_{\substack{\{u,v\}\subseteq V(G)\\ uv\in E(G)}} (d(u)d(v)-1)d(u,v) \\ &= \frac{1}{4}\mathrm{Gut}(G) - \frac{m}{4}. \end{aligned}$$

Also, we have

$$\sum_{u\in V(G)} \frac{d(u)(d(u)-1)}{2} = \frac{1}{2}M_1(G) - m.$$

Plugging these expressions into the inequality yields the bound.

The equality holds if and only if for every pair of incident edges the equality holds in (3) and for every pair of non-incident edges the equality holds in (2). The equality in (3) for two incident edges $e = ux$ and $f = uy$ implies $xy \in E(G)$. When applied to all edges incident to the same vertex and then for all vertices, this further implies $G = K_n$. ■

The upper bound from the previous theorem is similar to the bound established in [17] and it is obtained by a similar method, it is just a bit tighter. This tighter bound enables us to establish the upper bound on the ratio $W(L(G))/W(G)$ in terms of the maximum and minimum degree of the graph.

Lemma 2 *For a graph G on n vertices with maximum degree Δ and minimum degree δ it holds that*

$$\frac{W(L(G))}{W(G)} \leq \frac{1}{2n\,(n-1)} \left((n-1)^2\Delta^2 - \delta^2\right)$$

with equality if and only if $G = K_n$.

Proof. Using Theorem 1 we have

$$W(L(G)) \leq \frac{1}{4}\mathrm{Gut}(G) - \frac{3}{8}M_1(G) + \frac{1}{2}m^2.$$

Since

$$m^2 = \frac{1}{4}(2m)^2 = \frac{1}{4}(\sum_{u\in V(G)} d(u))^2,$$

we further obtain

$$\begin{aligned} W(L(G)) &\leq \frac{1}{4}\mathrm{Gut}(G) - \frac{3}{8}\sum_{u\in V(G)} d^2(u) + \frac{1}{8}(\sum_{u\in V(G)} d(u))^2 \\ &= \frac{1}{4}\mathrm{Gut}(G) + \frac{1}{8}\left((\sum_{u\in V(G)} d(u))^2 - 3\sum_{u\in V(G)} d^2(u)\right) \\ &= \frac{1}{4}\mathrm{Gut}(G) + \frac{1}{4}\left(\sum_{\{u,v\}\subseteq V(G)} d(u)d(v) - \sum_{u\in V(G)} d^2(u)\right). \end{aligned}$$

Let w be a vertex from G such that $d(w) = \delta$ and then notice the following

$$\begin{aligned}
\sum_{\{u,v\}\subseteq V(G)} d(u)d(v) - \sum_{u\in V(G)} d^2(u) &= \sum_{u\in V(G)\setminus\{w\}} d(u)d(w) \\
&+ \sum_{\{u,v\}\subseteq V(G)\setminus\{w\}} d(u)d(v) - \sum_{u\in V(G)} d^2(u) \\
&= \sum_{u\in V(G)\setminus\{w\}} d(u)\delta + \sum_{\{u,v\}\subseteq V(G)\setminus\{w\}} d(u)d(v) - \sum_{u\in V(G)} d^2(u) \\
&\le \sum_{\{u,v\}\subseteq V(G)\setminus\{w\}} d(u)d(v) - d(w)^2 \\
&\le \binom{n-1}{2}\Delta^2 - \delta^2.
\end{aligned}$$

Therefore, we have

$$\frac{W(L(G))}{W(G)} \le \frac{1}{4}\frac{\mathrm{Gut}(G)}{W(G)} + \frac{1}{4W(G)}\left(\binom{n-1}{2}\Delta^2 - \delta^2\right),$$

where we plug

$$\frac{\mathrm{Gut}(G)}{W(G)} \le \Delta^2 \quad \text{and} \quad W(G) \ge \binom{n}{2}$$

which yields the desired bound. The equality holds if and only if at every step we have equality, so Theorem 1 implies the equality holds only for $G = K_n$. ■

We can now establish the following theorem, which is the main result of the paper.

Theorem 3 *For a graph G on n vertices it holds that*

$$\frac{W(L(G))}{W(G)} \le \binom{n-1}{2}$$

with equality if and only if $G = K_n$.

Proof. Let us first consider the complete graph K_n. We have $W(K_n) = \binom{n}{2}$. As for the line graph, notice that $d_{L(K_n)}(e, f) = 2$ except when e and f share an end-vertex in which case $d_{L(K_n)}(e, f) = 1$, so we conclude that

$$\frac{W(L(K_n))}{W(K_n)} = \frac{2\binom{\binom{n}{2}}{2} - n\binom{n-1}{2}}{\binom{n}{2}} = \frac{\binom{n}{2}(\binom{n}{2}-1) - \binom{n}{2}(n-2)}{\binom{n}{2}} = \binom{n-1}{2}.$$

Therefore, the bound holds for $G = K_n$ with equality.

Again, let δ and Δ respectively denote the minimum and maximum degree of a graph G. For a graph G with $\Delta \le n-2$, Lemma 2 implies

$$\frac{W(L(G))}{W(G)} \le \frac{1}{2n\,(n-1)}\left((n-1)^2(n-2)^2 - 1^2\right) < \binom{n-1}{2}.$$

Assume therefore that $G \neq K_n$ is a graph with $\Delta = n-1$ and let u be the vertex such that $d(u) = \Delta = n-1$. Let v be a vertex in G such that $d(v) = \delta < n-1$ and let w be a vertex in G non adjacent to v. Notice that $d(w) \leq n-2$. Let G' be the graph obtained from G by adding the edge $g = vw$ to it. For a pair of edges $\{e, f\} \subseteq E(G)$ we denote

$$\Delta(e, f) = d_{L(G')}(e, f) - d_{L(G)}(e, f),$$

so we have

$$W(L(G')) - W(L(G)) = \sum_{\{e,f\} \subseteq E(G)} \Delta(e, f) + \sum_{e \in E(G)} d_{L(G')}(e, g).$$

Notice that for e, f from $E(G)$ it holds that $\Delta(e, f) = 0$ except possibly when e is incident to v and f is incident to w in which case $\Delta(e, f) = -1$. Therefore,

$$\sum_{\{e,f\} \subseteq E(G)} \Delta(e, f) \geq -d(v)d(w) \geq -(n-2)\delta.$$

Furthermore, notice that $d_{L(G')}(e, g) = 1$ only if e is incident to v or w, otherwise $d_{L(G')}(e, g) \geq 2$. From this we obtain

$$\begin{aligned}\sum_{e \in E(G)} d_{L(G')}(e, g) &\geq 2\,|E(G)| - d(v) - d(w) = \sum_{x \in V(G)} d(x) - \delta - d(w) \\ &\geq \delta + 1 + \sum_{x \in V(G) \setminus \{u,w\}} d(x) - \delta > (n-2)\delta.\end{aligned}$$

Therefore, we obtain $W(L(G')) - W(L(G)) > 0$ which further implies

$$\frac{W(L(G'))}{W(G')} > \frac{W(L(G))}{W(G')} \geq \frac{W(L(G))}{W(G)}.$$

If $G' = K_n$, we are done, otherwise the edge addition can be repeated until K_n is obtained.
■

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