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Terminal Wiener Index of Line Graphs

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Abstract

The terminal Wiener index of a graph is defined as the sum of the distances between the pendent vertices of a graph. In this paper we obtain results for the terminal Wiener index of line graphs.

1. Introduction

Let G be a connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \ldots, e_m\}$. The *degree* of a vertex v in G is the number of edges incident to it and is denoted by $deg_G(v)$. If $deg_G(v) = 1$ then v is called a *pendent vertex*. An edge $e = uv$ of a graph G is called a *pendent edge* if $deg_G(u) = 1$ or $deg_G(v) = 1$. Two edges are said to be *independent* if they are not adjacent to each other. An edge e is called a *bridge* if removal of e from G increases the number of components. The *distance* between the vertices v_i and v_j in G is equal to the length of a shortest path joining them and is denoted by $d(v_i, v_j|G)$.

The *Wiener index* $W = W(G)$ of a graph G is defined as the sum of the distances between all pairs of vertices of G, that is,

$$W = W(G) = \sum_{1 \leq i < j \leq n} d(v_i, v_j | G) \ .$$

This molecular structure descriptor was conceived by Harold Wiener [21] in 1947. For details on its chemical applications and mathematical properties one may refer to [4,5,8, 13,14,18,20] and the references cited therein.

If G has k pendent vertices labeled by $v_1, v_2, \ldots, v_k$, then its *terminal distance matrix* is the square matrix of order k whose (i,j)-th entry is $d(v_i, v_j|G)$. Terminal distance matrices were used for modeling amino acid sequences of proteins and of the genetic code [10,16,17].

The *terminal Wiener index* $TW(G)$ of a connected graph G is defined as the sum of the distances between all pairs of its pendent vertices.

Thus, if $V_T(G) = \{v_1, v_2, \ldots, v_k\}$ is the set of all pendent vertices of G, then

$$TW(G) = \sum_{\{v_i,v_j\} \subseteq V_T(G)} d(v_i, v_j|G) = \sum_{1 \leq i < j \leq k} d(v_i, v_j|G) \ .$$

This distance–based molecular structure descriptor was recently put forward by Gutman, Furtula and Petrović [7]. The same idea was, independently, developed by Székely, Wang, and Wu [19].

If the graph G has no pendent vertex or has only one pendent vertex, then $TW(G) = 0$. If G has at least two pendent vertices then $TW(G) \geq 1$. More details on the terminal Wiener index are found in the review [6] and in the recent papers [3,9].

Of the numerous results on the Wiener index of line graphs are we mention here [1,2,11,12,15,22]. In this paper we offer a few results on the terminal Wiener index of line graphs.

2. Terminal Wiener index of line graphs

The *line graph* of G, denoted by $L(G)$ is the graph whose vertices are the edges of G and two vertices of $L(G)$ are adjacent if and only if the corresponding edges are adjacent in G.

Observations

1. Let $e = uv$ be an edge of G such that $deg_G(u) = 1$ and $deg_G(v) = 2$. Then $deg_{L(G)}(e) = deg_G(u) + deg_G(v) - 2 = 1$. Therefore e is a pendent vertex of $L(G)$.

2. Let $e = uv$ be a pendent edge of G such that $deg_G(u) = 1$ and $deg_G(v) = 2$. Then v is a pendent vertex of G', where G' is the graph obtained by removing pendent vertices of G.

We define the set $D_2(G)$ as

$$D_2(G) = \{v \mid deg_G(v) = 2 \text{ and one neighbour of } v \text{ is pendent}\} .$$

Theorem 2.1. *Let G be a connected graph with $n \geq 4$ vertices and let $D_2(G) = \{v_1, v_2, \ldots, v_q\}$. Then*

$$TW(L(G)) = \sum_{1 \leq i < j \leq q} d(v_i, v_j|G) + \frac{q(q-1)}{2} . \tag{1}$$

Proof. Let $E_k = \{e_1, e_2, \ldots, e_k\}$ be the set of pendent edges of G and $E_q = \{e_1, e_2, \ldots, e_q\}$ be the subset of E_k where for each $e_i \in E_q$, the edge e_i is incident to $v_i \in D_2(G)$, $i = 1, 2, \ldots, q$. Thus, if $e_i = uv \in E_q$ then $deg_G(u) = 1$ and $deg_G(v) = 2$ (or vice versa), $i = 1, 2, \ldots, q$.

Consider two edges $e_i = uv_i$ and $e_j = v_j w$ of E_q where $deg_G(u) = deg_G(w) = 1$ and $deg_G(v_i) = deg_G(v_j) = 2$, $i = 1, 2, \ldots, q$.

Therefore e_i and e_j are the pendent vertices of $L(G)$ and $d(e_i, e_j|L(G)) = d(v_i, v_j|G)+1$. Therefore

$$\begin{aligned} TW(L(G)) &= \sum_{1 \leq i < j \leq q} d(e_i, e_j|L(G)) = \sum_{1 \leq i < j \leq q} [d(v_i, v_j|G) + 1] \\ &= \sum_{1 \leq i < j \leq q} d(v_i, v_j|G) + \frac{q(q-1)}{2} . \qquad \square \end{aligned}$$

Corollary 2.2. $TW(L(G)) = 0$ *if and only if the graph G satisfies one of the following conditions. (i) G has no edge $e = uv$ where $deg_G(u) = 1$ and $deg_G(v) = 2$. (ii) G has only one edge $e = uv$ where $deg_G(u) = 1$ and $deg_G(v) = 2$. (iii) G has no pendent vertices. (iv) G has only one pendent vertex. (v) G has no vertex of degree* 2.

Theorem 2.3. *Let G be a connected graph with $n \geq 4$ vertices and G' be the graph obtained from G by removing pendent vertices of G. If p is the number of pendent vertices of G', then*

$$TW(L(G)) \leq TW(G') + \frac{p(p-1)}{2} \,.$$

Equality holds if and only if (i) $G = K_{1,n-1}$ or (ii) G has no bridge e such that one of the component of $G - e$ is $K_{1,s}$, $s \geq 2$ and $G \neq K_{1,n-1}$.

Proof. Let $D_2(G) = \{v_1, v_2, \ldots, v_q\}$. Then the number of pendent vertices of G' is at least q. Let p be the number of pendent vertices of G'. Then $p \geq q$. From Theorem 2.1,

$$\begin{aligned} TW(L(G)) &= \sum_{1\leq i<j\leq q} d(v_i, v_j|G) + \frac{q(q-1)}{2} \leq \sum_{\{u,v\}\subseteq V_T(G')} d(u, v|G') + \frac{p(p-1)}{2} \\ &= TW(G') + \frac{p(p-1)}{2} \,. \end{aligned}$$

For equality we consider the following cases:

Case 1. It is obvious that equality holds for $G = K_{1,n-1}$.

Case 2. If $G \neq K_{1,n-1}$ and if there is no edge e in G such that one of the components of $G - e$ is $K_{1,s}$, $s \geq 2$, then $q = p$. That is, the vertices of the set $D_2(G)$ become pendent in G'. Therefore

$$\sum_{1\leq i<j\leq p} d(v_i, v_j|G) = \sum_{\{v_i,v_j\}\subseteq V_T(G')} d(v_i, v_j|G') \,.$$

Substituting this in Eq. (1) we get

$$TW(L(G)) = \sum_{\{v_i,v_j\}\subseteq V_T(G')} d(v_i, v_j|G') + \frac{p(p-1)}{2} = TW(G') + \frac{p(p-1)}{2} \,.$$

Conversely, let G contain a bridge e such that one of the component of $G - e$ is $K_{1,s}$, $s \geq 2$. Then $p > q$ implying

$$\sum_{1\leq i<j\leq q} d(v_i, v_j|G) < \sum_{\{v_i,v_j\}\subseteq V_T(G')} d(v_i, v_j|G') \,. \tag{2}$$

From Eq. (1),

$$\begin{aligned} TW(L(G)) &= \sum_{1\leq i<j\leq q} d(v_i, v_j|G) + \frac{q(q-1)}{2} \\ &< \sum_{\{v_i,v_j\}\subseteq V_T(G')} d(v_i, v_j|G') + \frac{p(p-1)}{2} \qquad \text{by Eq. (2) and } q < p \\ &= TW(G') + \frac{p(p-1)}{2} \end{aligned}$$

which is a contradiction. This completes the proof. $\square$

Corollary 2.4. *Let G be a connected graph with $n \geq 4$ vertices and G' be the graph obtained from G by removing pendent vertices. Let p be the number of pendent vertices of G'. If all pendent edges of G are mutually independent, then*

$$TW(L(G)) = TW(G') + \frac{p(p-1)}{2} .$$

Proof. Follows from the equality part of Theorem 2.3. $\square$

3. Terminal Wiener index of line graphs of some graphs

Let the vertices of G be $v_1, v_2, \ldots, v_n$ then G^+ is the graph obtained from G by adding n new vertices $v'_1, v'_2, \ldots, v'_n$ and joining v'_i to v_i by an edge, $i = 1, 2, \ldots, n$.

Theorem 3.1. *If G has k pendent vertices, then $L(G^+)$ also has k pendent vertices.*

Proof. If G has n vertices of which k are pendent vertices, then G^+ has n pendent edges of which k pendent edges say $e_1, e_2, \ldots, e_k$ are such that for each $e_i = uv$, $i = 0, 1, 2, \ldots, k$, $deg_{G^+}(u) = 1$ and $deg_{G^+}(v) = 2$.

Therefore $deg_{L(G^+)}(e_i) = deg_{G^+}(u) + deg_{G^+}(v) - 2 = 1$, $i = 0, 1, 2, \ldots, k$. Therefore $L(G^+)$ has k pendent vertices. $\square$

Theorem 3.2. *Let G be a connected graph with k pendent vertices, then*

$$TW(L(G^+)) = TW(G) + \frac{k(k-1)}{2} .$$

Proof. If n is the number of vertices of G, then G^+ has n pendent edges of which k pendent edges say $e_1, e_2, \ldots, e_k$ are such that for each $e_i = uv$, $i = 0, 1, 2, \ldots, k$, $deg_{G^+}(u) = 1$ and $deg_{G^+}(v) = 2$, since G has k pendent vertices. Removing pendent vertices of G^+ we get the graph G. Knowing that the pendent edges of G^+ are mutually independent, from Corollary 2.4,

$$TW(L(G^+)) = TW(G) + \frac{k(k-1)}{2} . \qquad \square$$

Let K_n and S_n be the *complete graph* and *star*, respectively, on n vertices.

Corollary 3.3. $TW(L(S_n^+)) = TW(K_{n-1}^+)$.

Proof. Star S_n has $n-1$ pendent vertices. Therefore from Theorem 3.2,

$$\begin{aligned} TW(L(S_n^+)) &= TW(S_n) + \frac{(n-1)(n-2)}{2} \\ &= \frac{2(n-1)(n-2)}{2} + \frac{(n-1)(n-2)}{2} \\ &= \frac{3(n-1)(n-2)}{2} \\ &= TW(K_{n-1}^+)\ . \qquad \square \end{aligned}$$

Theorem 3.4. *Let G be a connected graph with k pendent vertices and $H_t = L(H_{t-1}^+)$, $t = 1, 2, \ldots$, where $H_0 = G$ and $H_1 = L(G^+)$, then*

$$TW(H_t) = TW(G) + \frac{tk(k-1)}{2}\ .$$

Proof. As G has k pendent vertices, from Theorem 3.1, the graph H_t also has k pendent vertices, $t = 1, 2, \ldots$. From Theorem 3.2,

$$TW(H_1) = TW(L(G^+)) = TW(G) + \frac{k(k-1)}{2}\ .$$

By induction, let

$$TW(H_{t-1}) = TW(G) + \frac{(t-1)k(k-1)}{2}\ .$$

Therefore

$$\begin{aligned} TW(H_t) &= TW(L(H_{t-1}^+)) \\ &= TW(H_{t-1}) + \frac{k(k-1)}{2} \\ &= TW(G) + \frac{(t-1)k(k-1)}{2} + \frac{k(k-1)}{2} \\ &= TW(G) + \frac{tk(k-1)}{2}\ . \qquad \square \end{aligned}$$

The *subdivision graph* $S(G)$ is obtained from G by inserting a new vertex of degree 2 on each edge of G. The graph $S_l(G)$ is obtained from G by inserting l new vertices of degree 2 on each edge of G. Thus $S_1(G) = S(G)$.

Theorem 3.5. *Let G be a connected graph with k pendent vertices. Then*

$$TW(L(S_l(G)) = (l+1)TW(G) - \frac{k(k-1)}{2}\ , \quad l \geq 1\ .$$

Proof. If G has k pendent vertices then $S_l(G)$ also has k pendent vertices. That is $S_l(G)$ has k pendent edges.

If u and v are pendent vertices of G, then u and v are pendent vertices of $S_l(G)$. Let u' and v' be the subdivision vertices where u' is adjacent to u and v' is adjacent to v in $S_l(G)$, where u and v are pendent vertices of G. Let $(S_l(G))'$ be the graph obtained by removing all pendent vertices of $S_l(G)$. Therefore u' and v' are pendent vertices of $(S_l(G))'$ and $d(u', v'|(S_l(G))') = (l+1)d(u, v|G) - 2$. Since the pendent edges of $S_l(G)$ are mutually independent, from Corollary 2.4,

$$\begin{aligned}
TW(L(S_l(G)) &= TW((S_l(G))') + \frac{k(k-1)}{2} \\
&= \sum_{\{u',v'\}\subseteq V_T((S_l(G))')} d(u', v'|(S_l(G))') + \frac{k(k-1)}{2} \\
&= \sum_{\{u,v\}\subseteq V_T(G)} [(l+1)d(u, v|G) - 2] + \frac{k(k-1)}{2} \\
&= (l+1) \sum_{\{u,v\}\subseteq V_T(G)} d(u, v|G) - \frac{2k(k-1)}{2} + \frac{k(k-1)}{2} \\
&= (l+1)TW(G) - \frac{k(k-1)}{2}\,. \qquad \square
\end{aligned}$$

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