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ON THE WIENER INDEX OF A GRAPH

Harishchandra S. Ramane[1], Deepak S. Revankar[2], and Asha B. Ganagi[3]

[1]Department of Mathematics, Gogte Institute of Technology, Udyambag, Belgaum – 590008, India, hsramane@yahoo.com
[2]Department of Mathematics, Gogte Institute of Technology, Udyambag, Belgaum – 590008, India, revankards@rediffmail.com
[3]Department of Mathematics, Gogte Institute of Technology, Udyambag, Belgaum – 590008, India, abganagi@yahoo.co.in

Abstract. The Wiener index of a graph G, denoted by $W(G)$ is the sum of the distances between all (unordered) pairs of vertices of G. In this paper, we obtain the Wiener index of line graphs and some class of graphs.

Key words: Wiener index, line graph, distance, diameter.

Abstrak. Indeks Weiner dari suatu graf G, yang dinotasikan dengan $W(G)$ adalah jumlahan jarak antara semua pasangan (tak terurut) dari titik-titik G. Pada artikel ini, kami mendapatkan indeks Weiner dari graf garis dan beberapa kelas dari graf.

Kata kunci: Indeks Wiener, graf garis, jarak, diameter.

1. Introduction

Let G be a simple, connected, undirected 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 *distance* between two vertices v_i and v_j, denoted by $d(v_i, v_j)$ is the length of shortest path between the vertices v_i and v_j in G. The shortest $v_i - v_j$ path is often called a *geodesic*. The *diameter* $diam(G)$ of a connected graph G is the length of any longest geodesic. The *degree* of a vertex v_i in G is the number of edges incident to v_i and is denoted by $d_i = deg(v_i)$ [2, 11].

The *Wiener index* (or Wiener number) [18] of a graph G, denoted by $W(G)$ is the sum of the distances between all (unordered) pairs of vertices of G, that is

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

The Wiener index is a graph invariant that belongs to the molecules structure-descriptors called topological indices, which are used for the design of molecules with desired properties [16].

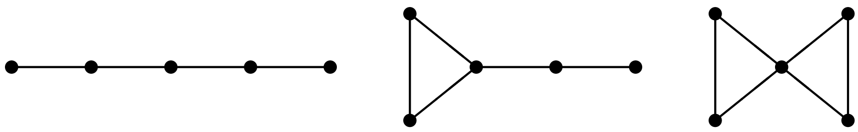
If $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_n$ be the eigenvalues of Laplacian Matrix [13] of a tree T, then [10, 12]

$$W(T) = n \sum_{i=1}^{n-1} \frac{1}{\mu_i}.$$

For details on Wiener index, see [4, 10, 14].

The line graph $L(G)$ of a graph G is a graph such that the vertices of $L(G)$ are the edges of G and two vertices of $L(G)$ are adjacent if and only if their corresponding edges in G share a common vertex [11]. The concept of line graph has various applications in physical chemistry [7, 9].

Let F_1 be the 5-vertex path, F_2 the graph obtained by identifying a vertex of a triangle with an end vertex of the 3-vertex path, and F_3 the graph obtained by identifying a vertex of a triangle with a vertex of another triangle (see Fig. 1).



F_1 F_2 F_3

Figure 1

Theorem 1.1. [15] *If $diam(G) \leq 2$ and none of the graphs F_1, F_2, F_3 of Fig. 1 is an induced subgraph of G then $diam(L(G)) \leq 2$.*

Recently there has been an interest in understanding the connection between $W(G)$ and $W(L(G))$.

Theorem 1.2. [1] *For every tree T on n vertices $W(L(T)) = W(T) - \binom{n}{2}$.*

Theorem 1.3. [6] *If G is connected graph with n vertices and m edges then*

$$W(L(G)) \geq W(G) - n(n-1) + \frac{m(m+1)}{2}.$$

Theorem 1.4. [8] *If G is connected unicyclic graph with n vertices then $W(L(G)) \leq W(G)$ with equality if and only if G is a cycle of length n.*

Theorem 1.5. [3] *Let G be a connected graph with minimum degree $\delta(G) \geq 2$ then $W(G) \leq W(L(G))$. Equality holds only for cycles.*

Graphs for which $W(G) = W(L(G))$ are considered in [3, 5].

In the sequel, in this paper we obtain some more results on the Weiner index of line graphs. Also, we obtain Wiener index of some class of graphs.

2. **Wiener Index of Line Graphs**

Theorem 2.1. *Let G be a connected graph with n vertices, m edges and $d_i = deg(v_i)$. If $diam(G) \leq 2$ and G does not contain F_i, $i = 1, 2, 3$ (of Fig. 1) as an induced subgraph then*

$$W(L(G)) = m^2 - \frac{1}{2}\sum_{i=1}^{n} d_i^2.$$

Proof. The number of vertices of $L(G)$ is $n_1 = m$ and the number of edges of $L(G)$ is $m_1 = -m + \frac{1}{2}\sum_{i=1}^{n} d_i^2$ [11].

If $diam(G) \leq 2$, then [17]

$$W(G) = n(n-1) - m \tag{1}$$

From Theorem 1.1, since $diam(G) \leq 2$ and G has no F_i, $i = 1, 2, 3$ as its induced subgraph then $diam(L(G)) \leq 2$. Therefore from Eq. (1),

$$\begin{aligned} W(L(G)) &= n_1(n_1 - 1) - m_1 \\ &= m(m-1) - \left[-m + \frac{1}{2}\sum_{i=1}^{n} d_i^2\right] \\ &= m^2 - \frac{1}{2}\sum_{i=1}^{n} d_i^2. \qquad \square \end{aligned}$$

Corollary 2.2. *If G is a connected r-regular graph on n vertices with $diam(G) \leq 2$ and none of F_i, $i = 1, 2, 3$ (of Fig. 1) as an induced subgraph of G then,*

$$W(L(G)) = \frac{nr^2(n-2)}{4}.$$

PROOF. Since G is an r-regular graph on n vertices, the number of edges of G is $m = nr/2$ and $d_i = deg(v_i) = r$. From Theorem 2.1,

$$\begin{aligned} W(L(G)) &= m^2 - \frac{1}{2}\sum_{i=1}^{n} d_i^2 \\ &= \left(\frac{nr}{2}\right)^2 - \frac{1}{2}\sum_{i=1}^{n} r^2 \\ &= \frac{n^2r^2}{4} - \frac{nr^2}{2} = \frac{nr^2(n-2)}{4}. \qquad \square \end{aligned}$$

Let $e = (uv)$ be an edge of a graph G where u and v are the end vertices of e. The degree of edge e is defined as $deg(e) = deg(u) + deg(v) - 2$.

Theorem 2.3. *Let G be a connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \ldots, e_m\}$. Let $d_i = deg(v_i)$. Then*

$$W(L(G)) \geq \sum_{i=1}^{n} \frac{d_i(d_i-1)}{2} + m(m-1) - \sum_{i=1}^{m} deg(e_i).$$

The equality holds if and only if $diam(G) \leq 2$ and none of the three graphs of Fig. 1 is an induced subgraph of G.

PROOF. If $d_i = deg(v_i)$ then for each vertex v_i there are d_i edges incident to v_i. These d_i edges form a complete graph on d_i vertices in $L(G)$. Which contributes $d_i(d_i-1)/2$ to the $W(L(G))$.

Consider an edge $e = (uv)$ which is adjacent to $deg(u) + deg(v) - 2 = deg(e)$ edges at u and v taken together. Hence the edge e is not adjacent to remaining $m-1-deg(e)$ edges of G. In $L(G)$ the distance between e and the remaining these $m-1-deg(e)$ vertices is more than 1. Hence each edge $e = (uv)$ contributes the distance at least $2(m-1-deg(e))$ in $L(G)$. Therefore

$$\begin{aligned} W(L(G)) &\geq \sum_{i=1}^{n} \frac{d_i(d_i-1)}{2} + \frac{1}{2} \sum_{e \in E(G)} 2(m-1-deg(e)) \\ &= \sum_{i=1}^{n} \frac{d_i(d_i-1)}{2} + \sum_{i=1}^{m} (m-1-deg(e_i)) \\ &= \sum_{i=1}^{n} \frac{d_i(d_i-1)}{2} + m(m-1) - \sum_{i=1}^{m} deg(e_i). \qquad \square \end{aligned}$$

For the equality:

If $diam(G) \leq 2$ and none of the three graphs of Fig. 1 is an induced subgraph of G, then from Theorem 1.1, $diam(L(G)) \leq 2$. Therefore as explained above, the distance between e and the remaining $m-1-deg(e)$ vertices in $L(G)$ is 2. Therefore

$$\begin{aligned} W(L(G)) &= \sum_{i=1}^{n} \frac{d_i(d_i-1)}{2} + \sum_{e \in E(G)} (m-1-deg(e)) \qquad (2) \\ &= \sum_{i=1}^{n} \frac{d_i(d_i-1)}{2} + m(m-1) - \sum_{i=1}^{m} deg(e_i) \end{aligned}$$

Conversely, the first part of Eq. (2) contributes the distance betwen the adjacent edges and the second part contributes the distance 2 between non adjacent edges. For this let e_i and e_j be nonadjacent edges in G. Since $d(e_i, e_j) = 2$ in $L(G)$, there is an edge e_k adjacent to e_i and e_j in G and none of the three graphs of Fig. 1 is an induced subgraph of G, $diam(G) \leq 2$. Hence G is required graph. $\square$

If G is an r-regular graph then $d_i = r$, $deg(e) = 2r-2$ and $m = nr/2$, so we have following corollary.

Corollary 2.4. *If G is a connected r-regular graph on n vertices then $W(LG)) \geq nr^2(n-2)/4$ with equality if and only if G is an r-regualr graph with $diam(G) \leq 2$ and none of the three graphs of Fig. 1 is an induced subgraph of G.*

Theorem 2.5. *If T is a tree with vertices $v_1, v_2, \ldots, v_n$ and $d_i = deg(v_i)$, $i = 1, 2, \ldots, n$ then*

$$W(L(T)) = \sum_{i=1}^{n} \frac{d_i(d_i-1)}{2} + \sum_{i<j} \left[1 + d(v_i, v_j)\right](d_i-1)(d_j-1). \qquad (3)$$

Proof. Edges of T will be the vertices of $L(T)$. For each vertex v_i there are d_i edges incident to it. These edges form a complete graph on d_i vertices in $L(T)$. Therfore the sum of the distances between these d_i vertices is

$$\binom{d_i}{2} = \frac{d_i(d_i-1)}{2}, \; i = 1, 2, \ldots, n. \tag{4}$$

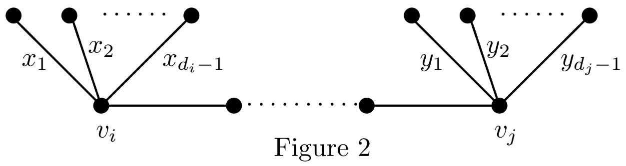


Figure 2

Now suppose v_i and v_j be the vertices of T and $d_i = deg(v_i)$ and $d_j = deg(v_j)$. Let $x_1, x_2, \ldots, x_{d_i-1}$ be the edges incident to v_i and $y_1, y_2, \ldots, y_{d_j-1}$ be the edges incident to v_j (Fig. 2). Where x_l, $(1 \le l \le d_i - 1)$ and y_k, $(1 \le k \le d_j - 1)$ do not have common vertex and these are not the edges of the path between v_i and v_j.

The distance between x_l and y_k in $L(T)$ is $1 + d(v_i, v_j)$.

The sum of the distances between all edges $x_1, x_2, \ldots, x_{d_i-1}$ incident to v_i and all edges $y_1, y_2, \ldots, y_{d_j-1}$ incidnet to v_j is

$$[1 + d(v_i, v_j)](d_i - 1)(d_j - 1). \tag{5}$$

Thus from Eq. (4) and Eq. (5),

$$W(L(T)) = \sum_{i=1}^{n} \frac{d_i(d_i-1)}{2} + \sum_{i<j} [1 + d(v_i, v_j)]\,(d_i - 1)(d_j - 1). \qquad \square$$

Theorem 2.6. *If T is a tree having k vertices with degree s and remaining with degree 1. Then*

$$W(L(T)) = \frac{ks(s-1)}{2} + (s-1)^2 \left[\binom{k}{2} + W(T') \right]$$

where T' is the tree obtained from T by removing all its end vertices.

Proof. The k vertices are of degree s and the remaining $n-k$ vertices are of degree 1. Say $deg(v_i) = s$ for $i = 1, 2, \ldots, k$ and $deg(v_i) = 1$ for $i = k+1, k+2, \ldots, n$. So $d_i - 1 = 0$ and $d_j - 1 = 0$ for $i, j = k+1, k+2, \ldots, n$. From Eq. (3),

$$
\begin{aligned}
W(L(T)) &= \sum_{i=1}^{k}\frac{s(s-1)}{2} + \sum_{1\le i<j\le k}[1+d(v_i,v_j)](s-1)(s-1)\\
&= \frac{ks(s-1)}{2} + \sum_{1\le i<j\le k}(s-1)^2 + \sum_{1\le i<j\le k}(s-1)^2 d(v_i,v_j)\\
&= \frac{ks(s-1)}{2} + (s-1)^2[(k-1)+(k-2)+\ldots+1] + (s-1)^2\sum_{1\le i<j\le k} d(v_i,v_j)\\
&= \frac{ks(s-1)}{2} + (s-1)^2\frac{(k-1)k}{2} + (s-1)^2 W(T')\\
&= \frac{ks(s-1)}{2} + (s-1)^2\left[\binom{k}{2} + W(T'))\right] \qquad \square
\end{aligned}
$$

3. **Wiener Index of Some Class of Graphs**

The clique of a graph G is the maximal complete induced subgraph of G [11].

Theorem 3.1. *Let G be a connected graph with n vertices having a clique K_k of order k. Let $G(n,k)$ be the graph obtained from G by removing the edges of K_k, $0 \le k \le n-1$. Then*

$$W(G(n,k)) \ge \frac{1}{2}[n(n-1)+k(k-1)].$$

The equality holds if and only if $G \cong K_n$, a complete graph on n vertices.

Proof. Let the vertices of G be $v_1, v_2, \ldots, v_n$. Without loss of generality, let the vertex set of the clique K_k of G be $S_1 = \{v_1, v_2, \ldots, v_k\}$ and the remaining vertices of G are $v_{k+1}, v_{k+2}, \ldots, v_n$.

In $G(n,k)$, $d(v_i,v_j) \ge 2$, if $v_i, v_j \in S_1$ and $d(v_i,v_j) \ge 1$, otherwise. So $\binom{k}{2}$ pairs of vertices are at distance greater than or equal to 2 and remaining $\binom{n}{2} - \binom{k}{2}$ pairs of vertices are at distance greater than or equal to 1. Therefore

$$
\begin{aligned}
W(G(n,k)) &= \sum_{i<j} d(v_i,v_j)\\
&\ge (2)\binom{k}{2} + (1)\left[\binom{n}{2} - \binom{k}{2}\right]\\
&= \frac{1}{2}[n(n-1)+k(k-1)].
\end{aligned}
$$

For the equality, if $G = K_n$, then in $G(n,k)$, $d(v_i, v_j) = 2$ if $v_i, v_j \in S_1$ and $d(v_i, v_j) = 1$, otherwise. So

$$\begin{aligned} W(G(n,k)) &= (2)\binom{k}{2} + (1)\left[\binom{n}{2} - \binom{k}{2}\right] \\ &= \frac{1}{2}[n(n-1) + k(k-1)]. \end{aligned}$$

Conversely, let $W(G(n,k)) = \frac{1}{2}[n(n-1) + k(k-1)]$.

Let $G \neq K_n$, then there exists at least one pair of vertices which are not adjacent. Let $v_1, v_2, \ldots, v_k$ be the vertices of the clique K_k of G. Let $v_{k+1}, v_{k+2}, \ldots, v_{k+l}$ be the vertices which are not adjacent among themselves in G, where $2 \leq l \leq n-k$.

Let $V_1 = \{v_1, v_2, \ldots, v_k\}$, $V_2 = \{v_{k+1}, v_{k+2}, \ldots, v_{k+l}\}$ and $V_3 = \{v_{k+l+1}, v_{k+l+2}, \ldots, v_n\}$.

In $G(n,k)$, $d(v_i, v_j) \geq 2$ if $v_i, v_j \in V_1$, $d(v_i, v_j) \geq 2$ if $v_i, v_j \in V_2$ and $d(v_i, v_j) \geq 1$, otherwise. Therefore

$$\begin{aligned} W(G(n,k)) &\geq (2)\binom{k}{2} + (2)\binom{l}{2} + (1)\left[\binom{n}{2} - \binom{k}{2} - \binom{l}{2}\right] \\ &= \frac{1}{2}[n(n-1) + k(k-1) + l(l-1)] \\ &\geq \frac{1}{2}[n(n-1) + k(k-1) + 2(2-1)] \qquad \text{since } l \geq 2 \\ &= \frac{1}{2}[n(n-1) + k(k-1) + 2)]. \end{aligned}$$

Which is a contradiction to $W(G(n,k)) = \frac{1}{2}[n(n-1) + k(k-1)]$. Hence $G = K_n$. □

Two subgraphs G_1 and G_2 of G with the vertex sets $V(G_1)$ and $V(G_2)$ respectively are said to be *independent* if $V(G_1) \cap V(G_2) = \phi$.

Theorem 3.2. *Let $(K_p)_i$, $i = 1, 2, \ldots, k$ be the k independent complete subgraphs on p vertices of K_n. Let $G(n,p,k)$ be the graph obtained from complete graph K_n by removing the edges of $(K_p)_i$, $i = 1, 2, \ldots, k$, $1 \leq k \leq \lfloor n/p \rfloor$ and $0 \leq p \leq n-1$, then*

$$W(G(n,p,k) = \frac{n(n-1) + kp(p-1)}{2}.$$

Proof. Let $(K_p)_1, (K_p)_2, \ldots, (K_p)_k$ be the independent subgraphs of K_n. Let $v_{(i-1)p+1}, v_{(i-1)p+2}, \ldots, v_{(i-1)p+p}$ be the vertices of $(K_p)_i$, $i = 1, 2, \ldots, k$. So in $G(n,p,k)$ there are $kp(p-1)/2$ pairs of vertices are at distance 2 and remaining $\binom{n}{2} - \frac{kp(p-1)}{2}$ pairs of vertices are at distance 1. Therefore

$$\begin{aligned} W(G(n,p,k) &= \sum_{i<j} d(v_i, v_j) \\ &= (2)\frac{kp(p-1)}{2} + (1)\left[\binom{n}{2} - \frac{kp(p-1)}{2}\right] \\ &= \frac{n(n-1)+kp(p-1)}{2}. \qquad \square \end{aligned}$$

Theorem 3.3. *Let e_i, $i = 1, 2, \ldots, k$, $0 \leq k \leq n-2$ be the edges of complete graph K_n incident to a vertex v of K_n. Let $K_n(k)$ be the graph obtained from K_n by removing the edges e_i, $i = 1, 2, \ldots, k$. Then*

$$W(K_n(k)) = \binom{n}{2} + k.$$

Proof. Let v is adjacent to $v_1, v_2, \ldots, v_k$ in the complete graph K_n. Therefore in $K_n(k)$ there are k pairs of vertices which are at distance 2 and remaining $\binom{n}{2} - k$ pairs of vertices are at distance 1. Therefore

$$\begin{aligned} W(K_n(k)) &= 2k + \left[\binom{n}{2} - k\right] \\ &= \binom{n}{2} + k. \qquad \square \end{aligned}$$

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