Wiener index of graphs in terms of eccentricities

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ABSTRACT

The Wiener index $W(G)$ of a connected graph G is defined as the sum of the distances between all unordered pairs of vertices of G. The eccentricity of a vertex v in G is the distance to a vertex farthest from v. In this paper we obtain the Wiener index of a graph in terms of eccentricities. Further we extend these results to the self-centered graphs.

Keywords: Wiener index, distance, eccentricity, radius, diameter, self-centered graph.

1. INTRODUCTION

The Wiener index $W(G)$ of a connected graph G is defined as the sum the distances between all unordered pairs of vertices of G. It was put forward by Harold Wiener [1]. The Wiener index is a graph invariant intensively studied both in mathematics and chemical literature. For details one may refer [2 – 13] and the reference cited there in.

Let G be a connected, simple graph with vertex set $V(G)$. The degree of a vertex v in G is the number of edges incident to it and is denoted by $deg(v)$. The distance between the vertices u and v, denoted by $d(u,v)$, is the length of the shortest path joining them. The eccentricity $e(v)$ of a vertex v is the distance to a vertex farthest from v, that is

$$e(v) = \max\{d(u,v) \mid u \in V(G)\}.$$

The radius $r(G)$ of a graph G is the minimum eccentricity of the vertices and the diameter $d(G)$ of G is the maximum eccentricity. A vertex v is called central vertex of G if $e(v) = r(G)$. A graph is called self-centered if every vertex is a central vertex. Thus in a self-centered graph $r(G) = d(G)$. An eccentric vertex of a vertex v is a vertex farthest away from v. An eccentric path of a vertex v denoted by $P(v)$ is a path of length $e(v)$ joining v and its eccentric vertex. There may exists more than one eccentric path for a given vertex.

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If $v_1, v_2, \dots, v_n$ are the vertices of graph G then the Wiener index of G is defined as

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

The distance number of a vertex v_i of a graph G denoted by $d(v_i \mid G)$ is defined as

$$d(v_i \mid G) = \sum_{j=1}^{n} d(v_i, v_j) .$$

Therefore

$$W(G) = \frac{1}{2} \sum_{i=1}^{n} d(v_i \mid G) .$$

In this paper we obtain the Wiener index in terms of eccentricities. For graph theoretic terminology we refer the book [14].

2. MAIN RESULTS

Theorem 2.1: Let G be a connected graph with n vertices, m edges and $e_i = e(v_i)$, $i = 1, 2, \dots, n$, then

$$W(G) \ge \frac{1}{2} \left[n(2n-1) - 2m + \sum_{i=1}^{n} \frac{e_i(e_i - 3)}{2} \right]. \qquad (1)$$

Equality holds if and only if for every vertex v_i of G, if $P(v_i)$ is one of the eccentric path of v_i, then for every $v_j \in V(G)$ which is not on $P(v_i)$, $d(v_i, v_j) \le 2$.

Proof: Let $P(v_i)$ be one of the eccentric path of $v_i \in V(G)$.

Let $A_1(v_i) = \{v_j \mid v_j$ is on eccentric path $P(v_i)$ of $v_i\}$,

$A_2(v_i) = \{v_j \mid v_j$ is adjacent to v_i and which is not on the eccentric path $P(v_i)$ of $v_i\}$,

$A_3(v_i) = \{v_j \mid v_j$ is not adjacent to v_i and not on the eccentric path $P(v_i)$ of $v_i\}$.

Clearly $A_1(v_i) \cup A_2(v_i) \cup A_3(v_i) = V(G)$ and

$|A_1(v_i)| = e_i + 1$, $|A_2(v_i)| = deg(v_i) - 1$, $|A_3(v_i)| = n - e_i - deg(v_i)$.

Now $$\sum_{v_j \in A_1(v_i)} d(v_i, v_j) = 1 + 2 + \cdots + e_i = \frac{e_i(e_i + 1)}{2},$$

$$\sum_{v_j \in A_2(v_i)} d(v_i, v_j) = deg(v_i) - 1,$$

$$\sum_{v_j \in A_3(v_i)} d(v_i, v_j) \ge 2(n - e_i - deg(v_i)) .$$

Therefore,

$$d(v_i\,|\,G)=\sum_{j=1}^{n}d(v_i,v_j)$$
$$=\sum_{v_j\in A_1(v_i)}d(v_i,v_j)+\sum_{v_j\in A_2(v_i)}d(v_i,v_j)+\sum_{v_j\in A_3(v_i)}d(v_i,v_j)$$
$$\geq\frac{e_i(e_i+1)}{2}+deg(v_i)-1+2(n-e_i-deg(v_i))$$
$$=2n-deg(v_i)-1+\frac{e_i(e_i-3)}{2}.$$

Therefore,

$$W(G)=\frac{1}{2}\sum_{i=1}^{n}d(v_i\,|\,G)$$
$$\geq\frac{1}{2}\sum_{i=1}^{n}\left[2n-deg(v_i)-1+\frac{e_i(e_i-3)}{2}\right]$$
$$=\frac{1}{2}\left[2n^2-2m-n+\sum_{i=1}^{n}\frac{e_i(e_i-3)}{2}\right]$$
$$=\frac{1}{2}\left[n(2n-1)-2m+\sum_{i=1}^{n}\frac{e_i(e_i-3)}{2}\right].$$

For equality,

Let G be a graph and $P(v_i)$ be one of the eccentric paths of $v_i\in V(G)$. Let $A_1(v_i)$, $A_2(v_i)$ and $A_3(v_i)$ be the sets as defined in the first part of the proof of this theorem.

Let $d(v_i, v_j) = 2$, where $v_j\in A_3(v_i)$.

Therefore $\sum_{v_j\in A_3(v_i)}d(v_i,v_j)=2(n-e_i-deg(v_i))$,

$$\sum_{v_j\in A_1(v_i)}d(v_i,v_j)=\frac{e_i(e_i+1)}{2}\quad\text{and}\quad\sum_{v_j\in A_2(v_i)}d(v_i,v_j)=deg(v_i)-1$$

Thus

$$d(v_i\,|\,G)=\sum_{j=1}^{n}d(v_i,v_j)$$
$$=\sum_{v_j\in A_1(v_i)}d(v_i,v_j)+\sum_{v_j\in A_2(v_i)}d(v_i,v_j)+\sum_{v_j\in A_3(v_i)}d(v_i,v_j)$$
$$=\frac{e_i(e_i+1)}{2}+deg(v_i)-1+2(n-e_i-deg(v_i))$$
$$=2n-deg(v_i)-1+\frac{e_i(e_i-3)}{2}.$$

Hence

$$W(G)=\frac{1}{2}\sum_{i=1}^{n}d(v_i\,|\,G)$$
$$=\frac{1}{2}\sum_{i=1}^{n}\left[2n-deg(v_i)-1+\frac{e_i(e_i-3)}{2}\right]$$
$$=\frac{1}{2}\left[2n^2-2m-n+\sum_{i=1}^{n}\frac{e_i(e_i-3)}{2}\right]$$
$$=\frac{1}{2}\left[n(2n-1)-2m+\sum_{i=1}^{n}\frac{e_i(e_i-3)}{2}\right].$$

Conversely,

Suppose G is not such graph as defined in the equality part of this theorem. Then there exist at least one vertex $v_j \in A_3(v_i)$ such that $d(v_i, v_j) \geq 3$. Let $A_3(v_i)$ be partitioned into two sets $A_{31}(v_i)$ and $A_{32}(v_i)$, where

$A_{31}(v_i) = \{v_j \mid v_j$ is not adjacent to v_i, not on the eccentric path $P(v_i)$ of v_i and $d(v_i, v_j) = 2\}$

$A_{32}(v_i) = \{v_j \mid v_j$ is not adjacent to v_i, not on the eccentric path $P(v_i)$ of v_i and $d(v_i, v_j) \geq 3\}$.

Let $|A_{32}(v_i)| = l \geq 1$. So, $|A_{31}(v_i)| = n - e_i - deg(v_i) - l$.

Therefore $\sum_{v_j\in A_1(v_i)} d(v_i,v_j)=\frac{e_i(e_i+1)}{2}$, $\sum_{v_j\in A_2(v_i)} d(v_i,v_j)=deg(v_i)-1$,

$\sum_{v_j\in A_{31}(v_i)} d(v_i,v_j)=2(n-e_i-deg(v_i)-l)$ and $\sum_{v_j\in A_{32}(v_i)} d(v_i,v_j)\geq 3l$.

Therefore

$$d(v_i\,|\,G)=\sum_{j=1}^{n}d(v_i,v_j)$$
$$=\sum_{v_j\in A_1(v_i)}d(v_i,v_j)+\sum_{v_j\in A_2(v_i)}d(v_i,v_j)+\sum_{v_j\in A_{31}(v_i)}d(v_i,v_j)+\sum_{v_j\in A_{32}(v_i)}d(v_i,v_j)$$
$$\geq\frac{e_i(e_i+1)}{2}+deg(v_i)-1+2(n-e_i-deg(v_i)-l)+3l$$
$$=2n-deg(v_i)-1+\frac{e_i(e_i-3)}{2}+l\,.$$

Therefore

$$W(G)=\frac{1}{2}\sum_{i=1}^{n}d(v_i\,|\,G)$$
$$\geq\frac{1}{2}\sum_{i=1}^{n}\left[2n-deg(v_i)-1+\frac{e_i(e_i-3)}{2}+l\right]$$
$$=\frac{1}{2}\left[2n^2-2m-n+\sum_{i=1}^{n}\frac{e_i(e_i-3)}{2}+nl\right]$$

$$\geq \frac{1}{2}\left[n(2n-1)-2m+\sum_{i=1}^{n}\frac{e_i(e_i-3)}{2}\right] \text{ as } l \geq 1, \text{ which is a contradiction.}$$

This contradiction proves the result. □

Corollary 2.2: Let G be a self-centered graph with n vertices, m edges and radius $r = r(G)$, then $W(G) \geq \frac{1}{2}\left[n(2n-1)-2m+\frac{nr(r-3)}{2}\right]$.

Equality holds if and only if for every vertex v_i of a self-centered graph G, if $P(v_i)$ is one of the eccentric path of v_i then for every $v_j \in V(G)$ which is not on the eccentric path $P(v_i)$, $d(v_i, v_j) \leq 2$.

Proof: For self-centered graph each vertex has same eccentricity equal to the radius r, that is, $e_i = e(v_i) = r$, $i = 1, 2, \dots, n$. Therefore from Eq. (1)

$$W(G) \geq \frac{1}{2}\left[n(2n-1)-2m+\sum_{i=1}^{n}\frac{r(r-3)}{2}\right]$$
$$= \frac{1}{2}\left[n(2n-1)-2m+\frac{nr(r-3)}{2}\right]$$

The proof of the equality part is similar to the proof of equality part of Theorem 1.1. □

Theorem 2.3: Let G be a connected graph with n vertices and $e_i = e(v_i)$, $i = 1, 2, \dots, n$, then

$$W(G) \geq \frac{1}{2}\left[n^2+\sum_{i=1}^{n}\frac{(e_i+1)(e_i-2)}{2}\right]. \qquad (2)$$

Equality holds if and only if for every vertex v_i of G, if $P(v_i)$ is one of the eccentric path of v_i, then for every $v_j \in V(G)$ which is not on $P(v_i)$, $d(v_i, v_j) = 1$.

Proof: Let $e_i = e(v_i)$, $i = 1, 2, \dots, n$ and $P(v_i)$ be one of the eccentric path of $v_i \in V(G)$.

Let $B_1(v_i) = \{v_j \mid v_j \text{ is on eccentric path } P(v_i) \text{ of } v_i\}$,

$B_2(v_i) = \{v_j \mid v_j \text{ is not on the eccentric path } P(v_i) \text{ of } v_i\}$.

Clearly $B_1(v_i) \cup B_2(v_i) = V(G)$ and

$|B_1(v_i)| = e_i + 1$, $|B_2(v_i)| = n - e_i - 1$.

Now $$\sum_{v_j \in B_1(v_i)} d(v_i, v_j) = 1+2+\cdots+e_i = \frac{e_i(e_i+1)}{2},$$

$$\sum_{v_j \in B_2(v_i)} d(v_i, v_j) \geq 1(n-e_i-1),$$

Therefore

$$d(v_i \mid G) = \sum_{j=1}^{n} d(v_i, v_j)$$
$$= \sum_{v_j \in B_1(v_i)} d(v_i, v_j) + \sum_{v_j \in B_2(v_i)} d(v_i, v_j)$$
$$\geq \frac{e_i(e_i+1)}{2} + n - e_i - 1$$
$$= n + \frac{(e_i-2)(e_i+1)}{2}.$$

Therefore

$$W(G) = \frac{1}{2}\sum_{i=1}^{n} d(v_i \mid G)$$
$$\geq \frac{1}{2}\sum_{i=1}^{n}\left[n + \frac{(e_i-2)(e_i+1)}{2}\right]$$
$$= \frac{1}{2}\left[n^2 + \sum_{i=1}^{n}\frac{(e_i-2)(e_i+1)}{2}\right].$$

For equality,

Let G be a graph and $P(v_i)$ be one of the eccentric paths of $v_i \in V(G)$. Let $B_1(v_i)$ and $B_2(v_i)$ be the sets as defined in the first part of the proof of this theorem.

Let $d(v_i, v_j) = 1$, where $v_j \in B_2(v_i)$.

Therefore $\sum_{v_j \in B_2(v_i)} d(v_i, v_j) = n - e_i - 1$ and $\sum_{v_j \in B_1(v_i)} d(v_i, v_j) = \frac{e_i(e_i+1)}{2}$.

Therefore

$$d(v_i \mid G) = \sum_{j=1}^{n} d(v_i, v_j)$$
$$= \sum_{v_j \in B_1(v_i)} d(v_i, v_j) + \sum_{v_j \in B_2(v_i)} d(v_i, v_j)$$
$$= \frac{e_i(e_i+1)}{2} + n - e_i - 1$$
$$= n + \frac{(e_i-2)(e_i+1)}{2}.$$

Therefore

$$W(G) = \frac{1}{2}\sum_{i=1}^{n} d(v_i \mid G)$$
$$= \frac{1}{2}\sum_{i=1}^{n}\left[n + \frac{(e_i-2)(e_i+1)}{2}\right]$$

$$= \frac{1}{2}\left[n^2 + \sum_{i=1}^{n}\frac{(e_i-2)(e_i+1)}{2}\right].$$

Conversely,

Suppose G is not such graph as defined in the equality part of this theorem. Then there exist at least one vertex $v_j \in B_2(v_i)$ such that $d(v_i, v_j) \geq 2$. Let $B_2(v_i)$ be partitioned into two sets $B_{21}(v_i)$ and $B_{22}(v_i)$, where

$B_{21}(v_i) = \{v_j \mid v_j$ is not on the eccentric path $P(v_i)$ of v_i and $d(v_i, v_j) = 1\}$

$B_{22}(v_i) = \{v_j \mid v_j$ is not on the eccentric path $P(v_i)$ of v_i and $d(v_i, v_j) \geq 2\}$.

Let $|B_{22}(v_i)| = l \geq 1$

Therefore $|B_{21}(v_i)| = n - e_i - 1 - l$.

Therefore $\sum_{v_j \in B_1(v_i)} d(v_i, v_j) = \frac{e_i(e_i+1)}{2}$, $\sum_{v_j \in B_{21}(v_i)} d(v_i, v_j) = n - e_i - 1 - l$ and $\sum_{v_j \in B_{22}(v_i)} d(v_i, v_j) \geq 2l$.

Therefore

$$\begin{aligned} d(v_i \mid G) &= \sum_{j=1}^{n} d(v_i, v_j) \\ &= \sum_{v_j \in B_1(v_i)} d(v_i, v_j) + \sum_{v_j \in B_{21}(v_i)} d(v_i, v_j) + \sum_{v_j \in B_{22}(v_i)} d(v_i, v_j) \\ &\geq \frac{e_i(e_i+1)}{2} + n - e_i - 1 - l + 2l \\ &= n + l + \frac{(e_i-2)(e_i+1)}{2}. \end{aligned}$$

Therefore

$$\begin{aligned} W(G) &= \frac{1}{2}\sum_{i=1}^{n} d(v_i \mid G) \\ &\geq \frac{1}{2}\sum_{i=1}^{n}\left[n + l + \frac{(e_i-2)(e_i+1)}{2}\right] \\ &\geq \frac{1}{2}\sum_{i=1}^{n}\left[n + 1 + \frac{(e_i-2)(e_i+1)}{2}\right] \text{ as } l \geq 1. \\ &= \frac{1}{2}\left[n(n+1) + \sum_{i=1}^{n}\frac{(e_i-2)(e_i+1)}{2}\right]. \end{aligned}$$

This is a contradiction. Hence the proof. □

If G is a self-centered graph then $e_i = e(v_i) = r(G)$ for all $i = 1, 2, \ldots, n$. Substituting this in Eq. (2) we get following corollary.

Corollary 2.4: Let G be a self-centered graph with n vertices and radius $r = r(G)$, then $W(G) \geq \frac{1}{2}\left[n^2 + \frac{n(r+1)(r-2)}{2}\right]$.

Equality holds if and only if for every vertex v_i of a self-centered graph G, if $P(v_i)$ is one of the eccentric path of v_i then for every $v_j \in V(G)$ which is not on the eccentric path $P(v_i)$, $d(v_i, v_j) = 1$.

Theorem 2.5: Let G be a connected graph with n vertices, m edges and $diam(G) = d$. Let $e_i = e(v_i)$, $i = 1, 2, \ldots, n$, then

$$W(G) \leq \frac{1}{2}\left[n(nd-1) - (1-d)2m + \sum_{i=1}^{n} \frac{e_i(e_i+1-2d)}{2}\right]. \tag{3}$$

Equality holds if and only if $diam(G) \leq 2$.

Proof: Let $P(v_i)$ be one of the eccentric path of $v_i \in V(G)$.

Let $A_1(v_i) = \{v_j \mid v_j$ is on the eccentric path $P(v_i)$ of $v_i\}$,

$A_2(v_i) = \{v_j \mid v_j$ is adjacent to v_i and which is not on the eccentric path $P(v_i)$ of $v_i\}$,

$A_3(v_i) = \{v_j \mid v_j$ is not adjacent to v_i and not on the eccentric path $P(v_i)$ of $v_i\}$.

Clearly $A_1(v_i) \cup A_2(v_i) \cup A_3(v_i) = V(G)$ and

$|A_1(v_i)| = e_i + 1$, $|A_2(v_i)| = deg(v_i) - 1$, $|A_3(v_i)| = n - e_i - deg(v_i)$.

Now

$$\sum_{v_j \in A_1(v_i)} d(v_i, v_j) = 1 + 2 + \cdots + e_i = \frac{e_i(e_i+1)}{2},$$

$$\sum_{v_j \in A_2(v_i)} d(v_i, v_j) = deg(v_i) - 1,$$

$$\sum_{v_j \in A_3(v_i)} d(v_i, v_j) \leq d(n - e_i - deg(v_i)).$$

Therefore

$$\begin{aligned} d(v_i \mid G) &= \sum_{j=1}^{n} d(v_i, v_j) \\ &= \sum_{v_j \in A_1(v_i)} d(v_i, v_j) + \sum_{v_j \in A_2(v_i)} d(v_i, v_j) + \sum_{v_j \in A_3(v_i)} d(v_i, v_j) \\ &\leq \frac{e_i(e_i+1)}{2} + deg(v_i) - 1 + d(n - e_i - deg(v_i)) \\ &= nd - 1 + (1-d)deg(v_i) + \frac{e_i(e_i+1-2d)}{2}. \end{aligned}$$

Therefore

$$W(G) = \frac{1}{2}\sum_{i=1}^{n} d(v_i \mid G)$$
$$\leq \frac{1}{2}\sum_{i=1}^{n}\left[nd - 1 + (1-d)deg(v_i) + \frac{e_i(e_i + 1 - 2d)}{2}\right]$$
$$= \frac{1}{2}\left[n(nd-1) + (1-d)2m + \sum_{i=1}^{n}\frac{e_i(e_i+1-2d)}{2}\right] \quad \text{since}$$
$$\sum_{i=1}^{n} deg(v_i) = 2m.$$

For equality,

Let $diam(G) \leq 2$.

<u>Case 1:</u> If $diam(G) = 1$ then $G = K_n$. Therefore $A_3(v_i) = \Phi$ and $e_i = e(v_i) = 1$, $i = 1, 2, \ldots, n$.

Therefore $W(G) = \frac{1}{2}\left[n(n-1) + \sum_{i=1}^{n}\frac{1(1+1-2)}{2}\right] = \frac{n(n-1)}{2}$.

<u>Case 2:</u> If $diam(G) = 2$, then for $v_j \in A_3(v_i)$, $d(v_i, v_j) = 2$.

Therefore $\sum_{v_j \in A_3(v_i)} d(v_i, v_j) = 2(n - e_i - deg(v_i))$.

Hence $W(G) = \frac{1}{2}\left[n(nd-1) + (1-d)2m + \sum_{i=1}^{n}\frac{e_i(e_i+1-2d)}{2}\right]$

$$= \frac{1}{2}\left[n(2n-1) - 2m + \sum_{i=1}^{n}\frac{e_i(e_i-3)}{2}\right].$$

Conversely,

$$d(v_i \mid G) = \sum_{j=1}^{n} d(v_i, v_j)$$
$$= \sum_{v_j \in A_1(v_i)} d(v_i, v_j) + \sum_{v_j \in A_2(v_i)} d(v_i, v_j) + \sum_{v_j \in A_3(v_i)} d(v_i, v_j) \quad (4)$$

The first summation of Eq. (4) contains the distance between v_i and the vertices on its eccentric path $P(v_i)$. Second summation of Eq. (4) contains the distance between v_i and its neighbor which are not on the eccentric path $P(v_i)$. The third summation of Eq. (4) contains the distance between v_i and a vertex which is neither adjacent to v_i nor on the eccentric path $P(v_i)$. Hence the equality in Eq. (4) holds if and only if $d = diam(G) \leq 2$. It is true for all $v_i \in V(G)$. Hence $diam(G) \leq 2$. □

Corollary 2.6: Let G be a self-centered graph with n vertices and radius $r = r(G)$, then

$$W(G) \leq \frac{1}{2}\left[n(nr-1) - \frac{(r-1)(nr+4m)}{2}\right].$$

Equality holds if and only if $diam(G) \leq 2$.

Proof: Proof follows by substituting $e_i = e(v_i) = r$, $i = 1, 2, \ldots, n$ in Eq. (3). □

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