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 \( v_1, v_2, \ldots, v_n \) are the vertices of graph \( G \) then the Wiener index of \( G \) is defined as
\[
W(G) = \sum_{1 \leq i < j \leq n} d(v_i, v_j).
\]

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 \( e_i = e(v_i), i = 1, 2, \ldots, n \), then
\[
W(G) \geq \frac{1}{2} \left[ n(2n-1) - 2m + \sum_{i=1}^{n} e_i(e_i - 3) \right].
\]  \hspace{1cm} (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 \( P(v_i) \), \( d(v_i, v_j) \leq 2 \).

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

Let \( A_1(v_i) = \{ v_j \mid v_j \text{ is on eccentric path } P(v_i) \text{ of } v_i \} \),
\( A_2(v_i) = \{ v_j \mid v_j \text{ is adjacent to } v_i \text{ and which is not on the eccentric path } P(v_i) \text{ of } v_i \} \),
\( A_3(v_i) = \{ v_j \mid v_j \text{ is not adjacent to } v_i \text{ and not on the eccentric path } P(v_i) \text{ of } v_i \} \).

Clearly \( A_1(v_i) \cup A_2(v_i) \cup A_3(v_i) = V(G) \) and
\[|A_1(v_i)| = e_i + 1, \quad |A_2(v_i)| = \text{deg}(v_i) - 1, \quad |A_3(v_i)| = n - e_i - \text{deg}(v_i)|.\]

Now
\[
\sum_{v_j \in A_1(v_i)} d(v_i, v_j) = 1 + 2 + \cdots + e_i = \frac{e_i(e_i + 1)}{2},
\]
\[
\sum_{v_j \in A_2(v_i)} d(v_i, v_j) = \text{deg}(v_i) - 1,
\]
\[
\sum_{v_j \in A_3(v_i)} d(v_i, v_j) \geq 2(n - e_i - \text{deg}(v_i)).
\]

Therefore,
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\[ d(v_i \mid G) = \sum_{j=1}^{n} d(v_i, v_j) \]

\[ = \sum_{v_j \in A_1(v_i)} d(v_i, v_j) + \sum_{v_j \in A_2(v_i)} d(v_i, v_j) + \sum_{v_j \in A_3(v_i)} d(v_i, v_j) \]

\[ \geq \frac{e_i(e_i + 1)}{2} + \text{deg}(v_i) - 1 + 2(n - e_i - \text{deg}(v_i)) \]

\[ = 2n - \text{deg}(v_i) - 1 + \frac{e_i(e_i - 3)}{2} \]

Therefore,

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

\[ \geq \frac{1}{2} \sum_{i=1}^{n} \left[ 2n - \text{deg}(v_i) - 1 + \frac{e_i(e_i - 3)}{2} \right] \]

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

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

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

\[ \sum_{v_j \in A_3(v_i)} d(v_i, v_j) = 2(n - e_i - \text{deg}(v_i)) , \]

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

Thus

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

\[ = \sum_{v_j \in A_1(v_i)} d(v_i, v_j) + \sum_{v_j \in A_2(v_i)} d(v_i, v_j) + \sum_{v_j \in A_3(v_i)} d(v_i, v_j) \]

\[ = \frac{e_i(e_i + 1)}{2} + \text{deg}(v_i) - 1 + 2(n - e_i - \text{deg}(v_i)) \]

\[ = 2n - \text{deg}(v_i) - 1 + \frac{e_i(e_i - 3)}{2} . \]

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

$$= \frac{1}{2} \sum_{i=1}^{n} \left[ 2n - \text{deg}(v_{i}) - 1 + \frac{e_{i}(e_{i} - 3)}{2} \right]$$

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

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

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

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

$A_{32}(v_{i}) = \{ v_{j} \mid v_{j} \text{ is not adjacent to } v_{i}, \text{ not on the eccentric path } P(v_{i}) \text{ of } v_{i} \text{ and } d(v_{i}, v_{j}) \geq 3 \}$. Let $|A_{32}(v_{i})| = l \geq 1$. So, $|A_{31}(v_{i})| = n - e_{i} - \text{deg}(v_{i}) - l$.

Therefore

$$\sum_{v_{i} \in A_{31}(v_{i}), v_{j} \in A_{32}(v_{i})} d(v_{i}, v_{j}) = e_{i}(e_{i} + 1) - 1,$$

$$\sum_{v_{i} \in A_{31}(v_{i}), v_{j} \in A_{32}(v_{i})} d(v_{i}, v_{j}) = \text{deg}(v_{i}) - 1,$$

$$\sum_{v_{i} \in A_{32}(v_{i})} d(v_{i}, v_{j}) = 2(n - e_{i} - \text{deg}(v_{i}) - l) \text{ and } \sum_{v_{i} \in A_{32}(v_{i})} d(v_{i}, v_{j}) \geq 3l.$$

Therefore

$$d(v_{i} \mid G) = \sum_{j=1}^{n} d(v_{i}, v_{j})$$

$$= \sum_{v_{i} \in A_{31}(v_{i})} d(v_{i}, v_{j}) + \sum_{v_{i} \in A_{31}(v_{i})} d(v_{i}, v_{j}) + \sum_{v_{i} \in A_{31}(v_{i})} d(v_{i}, v_{j}) + \sum_{v_{i} \in A_{31}(v_{i})} d(v_{i}, v_{j})$$

$$\geq \frac{e_{i}(e_{i} + 1)}{2} + \text{deg}(v_{i}) - 1 + 2(n - e_{i} - \text{deg}(v_{i}) - l) + 3l$$

$$= 2n - \text{deg}(v_{i}) - 1 + \frac{e_{i}(e_{i} - 3)}{2} + l.$$

Therefore

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

$$\geq \frac{1}{2} \sum_{i=1}^{n} \left[ 2n - \text{deg}(v_{i}) - 1 + \frac{e_{i}(e_{i} - 3)}{2} + l \right]$$

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

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, \( e_i = e(v_i) = r, \quad i = 1, 2, \ldots, n \). 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 \( e_i = e(v_i), \quad i = 1, 2, \ldots, n \), then

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

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 \( e_i = e(v_i), \quad i = 1, 2, \ldots, n \) and \( P(v_i) \) be one of the eccentric path of \( v_i \in V(G) \).

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

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

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

\[ |B_1(v_i)| = e_i + 1, \quad |B_2(v_i)| = n - e_i - 1. \]

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

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

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

This is a contradiction. Hence the proof. \(\square\)

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
\[ W(G) \leq \frac{1}{2} \left[ n(dn - 1) - (1 - d)2m + \sum_{i=1}^{n} e_i(e_i + 1 - 2d) \right]. \] (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 $A_1(v_i) = \{ v_j \mid v_j \text{ is on the eccentric path } P(v_i) \text{ of } v_i \}$,
$A_2(v_i) = \{ v_j \mid v_j \text{ is adjacent to } v_i \text{ and which is not on the eccentric path } P(v_i) \text{ of } v_i \}$,
$A_3(v_i) = \{ v_j \mid v_j \text{ is not adjacent to } v_i \text{ and not on the eccentric path } P(v_i) \text{ of } v_i \}$.
Clearly $A_1(v_i) \cup A_2(v_i) \cup A_3(v_i) = V(G)$ and
$|A_1(v_i)| = e_i + 1, \quad |A_2(v_i)| = deg(v_i) - 1, \quad |A_3(v_i)| = n - e_i - deg(v_i)$.

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

Therefore
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\[ W(G) = \frac{1}{2} \sum_{i=1}^{n} d(v_i | G) \]

For equality,

Let \( \text{diam}(G) \leq 2 \).

**Case 1:** If \( \text{diam}(G) = 1 \) then \( G = K_n \). Therefore \( A_2(v_i) = \Phi \) and \( e_i = e(v_i) = 1, i = 1, 2, \ldots, n. \)

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

**Case 2:** If \( \text{diam}(G) = 2 \), then for \( v_j \in A_3(v_i) \), \( d(v_i, v_j) = 2 \).

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

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

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

Conversely,

\[ d(v_i | G) = \sum_{j=1}^{n} d(v_i, v_j) \]

\[ = \sum_{v_j \in A_1(v_i)} d(v_i, v_j) + \sum_{v_j \in A_2(v_i)} d(v_i, v_j) + \sum_{v_j \in A_3(v_i)} d(v_i, v_j) \quad (4) \]

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 \( d = \text{diam}(G) \leq 2 \). It is true for all \( v_i \in V(G) \). Hence \( \text{diam}(G) \leq 2. \)

**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 $\text{diam}(G) \leq 2$.

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

**REFERENCES**