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FURTHER PROPERTIES OF REVERSE WIENER INDEX

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Abstract

The reverse Wiener index of a connected graph G is defined as

$$\Lambda = \Lambda(G) = \frac{1}{2}n(n-1)d - W(G)$$

where n, d and $W(G)$ are respectively the number of vertices, the diameter and the Wiener index of G. We determine the n-vertex trees with the k-th largest reverse Wiener indices for all k up to $\lfloor \frac{n}{2} \rfloor + 1$, the n-vertex unicyclic graphs with the k-th largest reverse Wiener indices for all k up to $n-3$ or nearly $n-3$, and the n-vertex bicyclic graphs with the k-th largest reverse Wiener indices for all k up to $\lfloor \frac{n-2}{2} \rfloor$.

1. INTRODUCTION

We consider simple graphs. The Wiener index $W(G)$ of a connected graph G is the sum of distances between all unordered pairs of vertices of G [1, 2]. It is one of the

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most thoroughly studied molecular–graph–based structure–descriptors that has been used to explain various chemical and physical properties of molecules and to correlate the structure of molecules with their biological activity [3–6]. Mathematical chemists have come up with various modifications, extensions and variants of this index, see, e.g., [7–14]. One such variant is the reverse Wiener index proposed by Balaban *et al.* [14].

Let G be a connected graph with n vertices. Then the reverse Wiener index of G is defined as [14]

$$\Lambda = \Lambda(G) = \frac{1}{2}n(n-1)d - W(G)$$

where d is the diameter of G. Comparisons between Λ and other structure–descriptors, especially Wiener index, were discussed in [14]. QSPR investigations in [14, 15] demonstrated that Λ is a useful structure–descriptor.

Let S_n and P_n be respectively the n-vertex star and the n-vertex path. Let T be a tree with $n > 4$ vertices, different from S_n and P_n. Zhang and Zhou [16] showed that $n-1 = \Lambda(S_n) < \Lambda(T) < \Lambda(P_n) = \frac{n(n-1)(n-2)}{3}$. Thus the reverse Wiener index can be used as a branching index. Cai and Zhou [17] established upper and lower bounds on the reverse Wiener index of a connected graph with given number of vertices, number of edges and diameter, and characterized trees that have the largest reverse Wiener index within some classes of trees.

Let G be a connected graph with vertices set $V(G)$. For $u, v \in V(G)$, we denote the distance between u and v in G by $d(u,v)$ and let $d(u,G) = \sum_{v \in V(G)} d(u,v)$.

Recall that a connected graph with n vertices and $n-1$ (resp. n, $n+1$) edges is known as a tree (resp. unicyclic graph, bicyclic graph).

In this paper, we report further properties of the reverse Wiener index. We determine the n-vertex trees with the k-th largest reverse Wiener indices for all k up to $\lfloor \frac{n}{2} \rfloor + 1$, the n-vertex unicyclic graphs with the k-th largest reverse Wiener indices for all k up to $n-3$ or nearly $n-3$, and the n-vertex bicyclic graphs with the k-th largest reverse Wiener indices for all k up to $\lfloor \frac{n-2}{2} \rfloor$.

2. REVERSE WIENER INDICES OF TREES

Let $P_{n,d,i}$ be the tree formed from the path P_{d+1} whose vertices are labelled consecutively as $v_0, \ldots, v_d$ by attaching $n-d-1$ pendent vertices to vertex v_i of the path, where $1 \le i \le d-1$ and $2 \le d \le n-2$ (see Fig. 1). Since $P_{n,d,i} = P_{n,d,d-i}$, we may require $1 \le i \le \lfloor \frac{d}{2} \rfloor$. If $d = n-1$, then $P_{n,n-1,i} = P_n$.

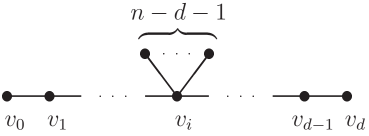

Fig. 1: The tree $P_{n,d,i}$.

Lemma 1. [16] *Let T be a tree with n vertices and diameter d, where $2 \leq d \leq n-2$. Then $\Lambda(T) \leq \Lambda\left(P_{n,d,\lfloor\frac{d}{2}\rfloor}\right)$ with equality if and only if $T = P_{n,d,\lfloor\frac{d}{2}\rfloor}$.*

Lemma 2. [16] *For $2 \leq d \leq n-2$, $\Lambda\left(P_{n,d,\lfloor\frac{d}{2}\rfloor}\right) < \Lambda\left(P_{n,d+1,\lfloor\frac{d+1}{2}\rfloor}\right)$.*

Theorem 3. *Let $n \geq 5$. Then*

$$\Lambda\left(P_{n,n-3,\lfloor\frac{n-3}{2}\rfloor}\right) < \Lambda\left(P_{n,n-2,1}\right) < \Lambda\left(P_{n,n-2,2}\right) < \cdots < \Lambda\left(P_{n,n-2,\lfloor\frac{n-2}{2}\rfloor}\right) < \Lambda(P_n)$$

and $\Lambda(T) < \Lambda\left(P_{n,n-3,\lfloor\frac{n-3}{2}\rfloor}\right)$ for any other n-vertex tree T.

Proof. Let T be a tree with n vertices and diameter d. Then $2 \leq d \leq n-1$.

If $d = n-1$, then $T = P_n$. Suppose that $d = n-2$. Then T is a tree $P_{n,n-2,i}$, where $1 \leq i \leq \lfloor\frac{n-2}{2}\rfloor$. Let v be the pendent vertex outside the diametrical path of T. It is easily seen that

$$\begin{aligned}
\Lambda(P_{n,n-2,i}) &= \frac{n(n-1)(n-2)}{2} - [W(P_{n-1}) + d(v, P_{n,n-2,i})] \\
&= \frac{n(n-1)(n-2)}{2} - \left[\frac{n(n-1)(n-2)}{6} + \sum_{s=1}^{i+1} s + \sum_{s=2}^{n-1-i} s\right] \\
&= \frac{n(n-1)(n-2)}{3} - \left(\sum_{s=1}^{i+1} s + \sum_{s=2}^{n-1-i} s\right) \\
&= \frac{n(n-1)(n-2)}{3} - \left[\frac{(i+1)(i+2)}{2} + \frac{(n-1-i)(n-i)}{2} - 1\right] \\
&= -i^2 + (n-2)i + \frac{n(n-1)(n-2)}{3} - \frac{n(n-1)}{2}.
\end{aligned}$$

Thus, $\Lambda(P_{n,n-2,i})$ is monotonically increasing for $1 \leq i \leq \lfloor\frac{n-2}{2}\rfloor$. It follows that the reverse Wiener indices of all n-vertices of diameter $n-2$ and $n-1$ may be ordered as:

$$\Lambda\left(P_{n,n-2,1}\right) < \Lambda\left(P_{n,n-2,2}\right) < \cdots < \Lambda\left(P_{n,n-2,\lfloor\frac{n-2}{2}\rfloor}\right) < \Lambda(P_n).$$

The last inequality follows from Lemma 2.

Now suppose that $d \leq n-3$. Note that

$$\begin{aligned}
& \Lambda\left(P_{n,n-3,i}\right) \\
= & \frac{n(n-1)(n-3)}{2} - \left[\frac{(n-1)(n-2)(n-3)}{6} + 2 + 2\sum_{s=1}^{i+1} s + 2\sum_{s=2}^{n-2-i} s\right] \\
= & -2i^2 + (2n-6)i + \frac{(n+1)(n-1)(n-3)}{3} - (n^2-3n+4)
\end{aligned}$$

for $1 \leq i \leq \lfloor \frac{n-3}{2} \rfloor$, and then

$$\begin{aligned}
& \Lambda\left(P_{n,n-2,1}\right) - \Lambda\left(P_{n,n-3,\lfloor \frac{n-3}{2} \rfloor}\right) \\
= & n-3-\frac{n(n-1)}{2} + \frac{n(n-1)(n-2)}{3} - \frac{(n+1)(n-1)(n-3)}{3} \\
& + n^2 - 3n + 4 + 2\left\lfloor \frac{n-3}{2} \right\rfloor^2 - 2(n-3)\left\lfloor \frac{n-3}{2} \right\rfloor \\
= & \left\lfloor \frac{5n-8}{2} \right\rfloor > 0\,.
\end{aligned}$$

Thus, by Lemma 1 and, if necessary ($d < n-3$), Lemma 2, we have $\Lambda(T) \leq \Lambda\left(P_{n,n-3,\lfloor \frac{n-3}{2} \rfloor}\right) < \Lambda\left(P_{n,n-2,1}\right)$ with the first equality holding if and only if $T = P_{n,n-3,\lfloor \frac{n-3}{2} \rfloor}$. Now the result follows. $\square$

By Theorem 3, the n-vertex trees with the k-th largest reverse Wiener indices for all k up to $\lfloor \frac{n}{2} \rfloor + 1$ are determined. In particular, for a tree T with n vertices different from P_n,

$$\Lambda(T) \leq \frac{n(n-1)(n-2)}{3} - \left\lfloor \frac{n^2+2n-3}{4} \right\rfloor$$

with equality if and only if $T = P_{n,n-2,\lfloor \frac{n-2}{2} \rfloor}$.

3. REVERSE WIENER INDICES OF UNICYCLIC GRAPHS

Let $G_{n,i}$ be the graph formed from the path P_{n-1} whose vertices are labelled consecutively as $v_0, \ldots, v_{n-2}$ by adding vertex v and edges vv_i, vv_{i+1}, where $0 \leq i \leq \lfloor \frac{n-3}{2} \rfloor$ and $H_{n,i}$ be the graph formed from the path P_{n-1} by adding vertex v and edges vv_i, vv_{i+2}, where $0 \leq i \leq \lfloor \frac{n-4}{2} \rfloor$. For simplicity, we write G_i for $G_{n,i}$ and H_i for $H_{n,i}$.

Lemma 4. *The reverse Wiener indices of G_i for $0 \leq i \leq \lfloor \frac{n-3}{2} \rfloor$ and H_i for $0 \leq i \leq \lfloor \frac{n-4}{2} \rfloor$ are given by:*

$$\begin{aligned}
\Lambda(G_i) &= -i^2 + (n-3)i + \frac{n(n-1)(n-2)}{3} - \frac{n^2-3n+4}{2}, \\
\Lambda(H_i) &= -i^2 + (n-4)i + \frac{n(n-1)(n-2)}{3} - \frac{n^2-5n+12}{2}.
\end{aligned}$$

Proof. From the definition of the reverse Wiener index,

$$\begin{aligned}
\Lambda(G_i) &= \frac{n(n-1)(n-2)}{2} - W(G_i) \\
&= \frac{n(n-1)(n-2)}{2} - [W(P_{n-1}) + d(v, G_i)] \\
&= \frac{n(n-1)(n-2)}{2} - \left[\frac{n(n-1)(n-2)}{6} + \sum_{s=1}^{i+1} s + \sum_{s=1}^{n-2-i} s\right] \\
&= \frac{n(n-1)(n-2)}{3} - \left[\frac{(i+1)(i+2)}{2} + \frac{(n-2-i)(n-1-i)}{2}\right] \\
&= -i^2 + (n-3)i + \frac{n(n-1)(n-2)}{3} - \frac{n^2-3n+4}{2},
\end{aligned}$$

$$\begin{aligned}
\Lambda(H_i) &= \frac{n(n-1)(n-2)}{2} - W(H_i) \\
&= \frac{n(n-1)(n-2)}{2} - [W(P_{n-1}) + d(v, H_i)] \\
&= \frac{n(n-1)(n-2)}{2} - \left[\frac{n(n-1)(n-2)}{6} + 2 + \sum_{s=1}^{i+1} s + \sum_{s=1}^{n-3-i} s\right] \\
&= \frac{n(n-1)(n-2)}{3} - \left[2 + \frac{(i+1)(i+2)}{2} + \frac{(n-3-i)(n-2-i)}{2}\right] \\
&= -i^2 + (n-4)i + \frac{n(n-1)(n-2)}{3} - \frac{n^2-5n+12}{2}. \quad \square
\end{aligned}$$

We need the following results from [17] (the first of which is a restatement of [18, Theorem 2]).

Lemma 5. [17] *Let G be a connected graph with n vertices and diameter d. Then*

$$\Lambda(G) \le \frac{n(n-1)d}{2} - \frac{d(d+1)(d+2)}{6} - \frac{n-d-1}{2}\left(n + \left\lfloor \frac{d^2+1}{2} \right\rfloor\right)$$

with equality if and only if there is a vertex v_0 such that the distance layers V_i, where V_i is a subset of the vertex set consisting of the vertices that are at distance i from v_0 for $i = 0, 1, \ldots, d$, fulfill the condition that the subgraphs induced $V_{i-1} \cup V_i$ are complete whenever $1 \le i \le d$ and all noncentral layers are trivial.

Lemma 6. [17] *For integers n and d with $1 \le d \le n-2$, let*

$$F(n,d) = \frac{n(n-1)d}{2} - \frac{d(d+1)(d+2)}{6} - \frac{n-d-1}{2}\left(n + \left\lfloor \frac{d^2+1}{2} \right\rfloor\right).$$

Then $F(n,d) < F(n,d+1)$.

Now we are ready to give the main result in this section.

Theorem 7. *Let $n \geq 5$. Then the reverse Wiener indices of graphs $G_0, \ldots, G_{\lfloor \frac{n-3}{2} \rfloor}$ and $H_0, \ldots, H_{\lfloor \frac{n-4}{2} \rfloor}$ may be ordered by the following relations:*

$$\Lambda(G_0) < \Lambda(G_1) < \cdots < \Lambda\left(G_{\lfloor \frac{n-3}{2} \rfloor}\right), \tag{1}$$

$$\Lambda(H_0) < \Lambda(H_1) < \cdots < \Lambda\left(H_{\lfloor \frac{n-4}{2} \rfloor}\right), \tag{2}$$

$$\Lambda\left(H_{\lfloor a_j \rfloor}\right) \leq \Lambda(G_j) < \Lambda\left(H_{\lfloor a_j \rfloor + 1}\right), \quad j = 1, \ldots, \left\lfloor \frac{n-3}{2} \right\rfloor \tag{3}$$

with left equality in (3) if and only if $a_j = \frac{n-4-\sqrt{(n-2j)^2-4(n-3j)}}{2}$ is a nonnegative integer, and $\Lambda(G) < \Lambda(G_0)$ for any other n-vertex unicyclic graph G.

Proof. Let G be a unicyclic graph with n vertices and diameter d. Then $2 \leq d \leq n-2$.

First suppose that $d = n-2$. Then G is either a graph G_j, where $0 \leq j \leq \lfloor \frac{n-3}{2} \rfloor$, or a graph H_i, where $0 \leq i \leq \lfloor \frac{n-4}{2} \rfloor$. By Lemma 4, $\Lambda(G_j)$ is monotonically increasing for $0 \leq j \leq \lfloor \frac{n-3}{2} \rfloor$ and $\Lambda(H_i)$ is monotonically increasing for $0 \leq i \leq \lfloor \frac{n-4}{2} \rfloor$, and thus we have (1) and (2). For $i \geq 1$ and $j \geq 1$, $\Lambda(H_i) \geq \Lambda(G_j)$ is equivalent to $-i^2 + (n-4)i + j^2 - (n-3)j + n - 4 \geq 0$, i.e., $i \geq a_j$, where $a_j = \frac{n-4-\sqrt{(n-2j)^2-4(n-3j)}}{2}$. Thus we have (3) with left equality if and only if a_j is a nonnegative integer.

Now suppose that $d \leq n-3$. Note that $\Lambda(G_0) = \frac{2n^3-9n^2+13n-12}{6}$, $F(n, n-3) = \frac{2n^3-9n^2+10n-24}{6}$ if n is even and $F(n, n-3) = \frac{2n^3-9n^2+10n-21}{6}$ if n is odd. Thus, $\Lambda(G_0) - F(n, n-3) = \lfloor \frac{n+4}{2} \rfloor > 0$, and then by Lemma 5 and, if necessary, Lemma 6, we have $\Lambda(G) \leq F(n, n-3) < \Lambda(G_0)$. $\square$

Suppose that $n \geq 6$. Setting $j = \lfloor \frac{n-3}{2} \rfloor$ in (3) and using (2) in Theorem 7, we have

$$\Lambda\left(G_{\lfloor \frac{n-3}{2} \rfloor}\right) \leq \left\{ \begin{array}{ll} \Lambda\left(H_{\lceil \frac{n-4-\sqrt{2n-8}}{2} \rceil}\right) & \text{if } n \text{ is even} \\ \Lambda\left(H_{\lceil \frac{n-4-\sqrt{2n-9}}{2} \rceil}\right) & \text{if } n \text{ is odd} \end{array} \right\} < \cdots < \Lambda\left(H_{\lfloor \frac{n-4}{2} \rfloor}\right)$$

with the first equality holding for even (resp. odd) n if and only if $\frac{n-4-\sqrt{2n-8}}{2}$ (resp. $\frac{n-4-\sqrt{2n-9}}{2}$) is a nonnegative integer. On the other hand, $a_1 = 0$ and for $2 \leq j \leq \lfloor \frac{n}{3} \rfloor$, $\lfloor a_j \rfloor = j-2$. Using (1), we have

$$\Lambda(G_0) < \Lambda(G_1) = \Lambda(H_0)$$

$$
\begin{aligned}
&< \Lambda(G_2) < \Lambda(H_1) < \Lambda(G_3) < \Lambda(H_2) < \cdots \\
&< \Lambda\left(G_{\lfloor\frac{n}{3}\rfloor-1}\right) < \Lambda\left(H_{\lfloor\frac{n}{3}\rfloor-2}\right) \leq \Lambda\left(G_{\lfloor\frac{n}{3}\rfloor}\right) \\
&< \Lambda\left(G_{\lfloor\frac{n}{3}\rfloor+1}\right) < \Lambda\left(H_{\lfloor\frac{n}{3}\rfloor-1}\right) .
\end{aligned}
$$

For example, the reverse Wiener indices of graphs $G_0, \ldots, G_{\lfloor\frac{n-3}{2}\rfloor}$ and $H_0, \ldots, H_{\lfloor\frac{n-4}{2}\rfloor}$ when $n = 5, \ldots, 10$ are ordered as:

$$
\begin{aligned}
\Lambda(G_0) < \Lambda(G_1) = \Lambda(H_0) \quad & \text{if } n = 5, \\
\Lambda(G_0) < \Lambda(G_1) = \Lambda(H_0) < \Lambda(H_1) \quad & \text{if } n = 6, \\
\Lambda(G_0) < \Lambda(G_1) = \Lambda(H_0) < \Lambda(G_2) < \Lambda(H_1) \quad & \text{if } n = 7, \\
\Lambda(G_0) < \Lambda(G_1) = \Lambda(H_0) < \Lambda(G_2) < \Lambda(H_1) < \Lambda(H_2) \quad & \text{if } n = 8, \\
\Lambda(G_0) < \Lambda(G_1) = \Lambda(H_0) < \Lambda(G_2) < \Lambda(G_3) = \Lambda(H_1) < \Lambda(H_2) \quad & \text{if } n = 9 \\
\Lambda(G_0) < \Lambda(G_1) = \Lambda(H_0) < \Lambda(G_2) < \Lambda(H_1) < \Lambda(G_3) < \Lambda(H_2) < \Lambda(H_3) \quad & \text{if } n = 10 .
\end{aligned}
$$

It follows that the n-vertex unicyclic graphs with the k-th largest reverse Wiener indices for all k up to $n-3$ or nearly $n-3$ are determined. In particular, for a unicyclic graph G with $n \geq 6$ vertices,

$$\Lambda(G) \leq \frac{n(n-1)(n-2)}{3} - 2 - \left\lfloor \frac{(n-1)^2}{4} \right\rfloor$$

with equality if and only if $G = H_{\lfloor\frac{n-4}{2}\rfloor}$.

4. REVERSE WIENER INDICES OF BICYCLIC GRAPHS

Let $L_{n,i}$ be the graph formed from the path P_{n-1} whose vertices are labelled consecutively as $v_0, \ldots, v_{n-2}$ by adding vertex v and edges vv_i, vv_{i+1} and vv_{i+2}, where $0 \leq i \leq \lfloor\frac{n-4}{2}\rfloor$.

Theorem 8. *Let $n \geq 5$. Then*

$$\Lambda\left(L_{n,0}\right) < \Lambda\left(L_{n,1}\right) < \cdots < \Lambda\left(L_{n,\lfloor\frac{n-4}{2}\rfloor}\right)$$

and $\Lambda(G) < \Lambda\left(L_{n,0}\right)$ for any other n-vertex bicyclic graph G.

Proof. Let G be a bicyclic graph with n vertices and diameter d. Then $2 \leq d \leq n-2$.

First suppose that $d = n-2$. Then G is a graph $L_{n,i}$, where $0 \leq i \leq \lfloor\frac{n-4}{2}\rfloor$. It is easily seen that

$$\Lambda\left(L_{n,i}\right) = \frac{n(n-1)(n-2)}{2} - \left[W(P_{n-1}) + d\left(v, L_{n,i}\right)\right]$$

$$= \frac{n(n-1)(n-2)}{2} - \left[\frac{n(n-1)(n-2)}{6} + 1 + \sum_{s=1}^{i+1} s + \sum_{s=1}^{n-3-i} s\right]$$
$$= \frac{n(n-1)(n-2)}{3} - \left[1 + \frac{(i+1)(i+2)}{2} + \frac{(n-3-i)(n-2-i)}{2}\right]$$
$$= -i^2 + (n-4)i + \frac{n(n-1)(n-2)}{3} - \frac{n^2-5n+10}{2}.$$

Thus, $\Lambda(L_{n,i})$ is monotonically increasing for $0 \le i \le \lfloor \frac{n-4}{2} \rfloor$. It follows that

$$\Lambda(L_{n,0}) < \Lambda(L_{n,1}) < \cdots < \Lambda\left(L_{n,\lfloor \frac{n-4}{2} \rfloor}\right).$$

Now suppose that $d \le n-3$. Note that $\Lambda(L_{n,0}) = \frac{2n^3-9n^2+19n-30}{6}$, $F(n, n-3) = \frac{2n^3-9n^2+10n-24}{6}$ if n is even and $F(n, n-3) = \frac{2n^3-9n^2+10n-21}{6}$ if n is odd. Thus, $\Lambda(L_{n,0}) - F(n, n-3) = \lfloor \frac{3n-2}{2} \rfloor > 0$, and then by Lemma 5 and, if necessary, Lemma 6, we have $\Lambda(G) \le F(n, n-3) < \Lambda(L_{n,0})$. The result follows. □

By Theorem 8, the n-vertex bicyclic graphs with the k-th largest reverse Wiener indices for all k up to $\lfloor \frac{n-2}{2} \rfloor$ are determined. In particular, for a bicyclic graph G with $n \ge 4$ vertices,

$$\Lambda(G) \le \frac{n(n-1)(n-2)}{3} - \left\lfloor \frac{n^2-2n+5}{2} \right\rfloor$$

with equality if and only if $G = L_{n,\lfloor \frac{n-4}{2} \rfloor}$.

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