Bounds on the Weighted Vertex PI Index of Cacti Graphs

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Abstract. The weighted vertex PI index of a graph G is defined by

$$PL_w(G) = \sum_{e=uv \in E(G)} (d_{G}(u) + d_{G}(v))(n_u(e|G) + n_v(e|G))$$

where $d_{G}(u)$ denotes the vertex degree of u and $n_u(e|G)$ denotes the number of vertices in G whose distance to the vertex u is smaller than the distance to the vertex v. A graph is a cactus if it is connected and all its blocks are either edges or cycles. In this paper, we give the upper and lower bounds on the weighted vertex PI index of cacti with n vertices and s cycles, and completely characterize the corresponding extremal graphs.

1. Introduction and background

Let $G = (V, E)$ be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. For vertices $u, v \in V$, the distance $d(u, v)$ is defined as the length of the shortest path between $u$ and $v$ in $G$. The length of a path or a cycle is the number of its edges. The minimum degree of a graph $G$ is denoted by $\delta(G)$. For more notations and terminologies that will be used, see [1].

A topological index is a real number related to a graph. It must be a structural invariant, i.e., it is preserved by every graph automorphisms. Several topological indices have been defined and many of them have found applications as means to model chemical, pharmaceutical and other properties of molecules.

The Wiener index is the first topological index based on graph distances [41] which was proposed in 1947. The Wiener index is defined as the sum of all distances between vertices of the graph under consideration. For more information on the Wiener index, the chemical applications of the index and its history, see [6, 7, 10, 11]. The PI index was proposed by Khadikar [16] in 2000. The PI index is the unique topological index related to equidistance of vertices or parallelism of edges. It is very simple to calculate and has discriminating power in some molecular graphs. The detailed applications of PI indices between chemistry and graph theory are investigated in [5, 13, 17, 18, 21, 25–27, 30, 31, 37, 44].

For each edge $e = uv \in E(G)$, let $n_u(e|G)$ be the number of vertices in $G$ whose distance to the vertex $u$ is smaller than the distance to the vertex $v$, and similarly, let $n_v(e|G)$ be the number of vertices in $G$ whose
distance to the vertex \( v \) is smaller than the distance to the vertex \( u \). The vertex PI index of a graph \( G \), proposed in [19], is defined as

\[
PL_v(G) = \sum_{e \in \text{deg}(G)} [n_u(e(G)) + n_v(e(G))].
\]

There are nice results regarding vertex PI index in the study of computational complexity and the intersection between graph theory and chemistry, see [3, 14, 19, 20, 22, 23, 32, 33, 36, 40]. One of the oldest degree-based graph invariants are the first Zagreb index [4, 9, 42], defined as follows:

\[
M_1(G) = \sum_{u \in V(G)} d^2(u),
\]

where \( d(u) \) denotes the vertex degree of \( u \). The vertex PI index, Zagreb indices and their variants have been used to study molecular complexity, chirality, in QSPR and QSAR analysis, see [9, 18].

In order to increase diversity for bipartite graphs, Ilić and Milosavljević [15] introduced the weighted vertex PI index as follows:

\[
PL_w(G) = \sum_{e \in \text{deg}(G)} (d(u) + d(v))(n_u(e(G)) + n_v(e(G))).
\]

This means that the weighted vertex PI index is directly connected to the first Zagreb index.

In [15], the authors show that among all connected graphs with \( n \) vertices, \( PL_w(G) \geq n(4n - 6) \), with equality holds if and only if \( G \cong P_n \). For any graph \( G \) with \( n \) vertices and \( m \) edges [19], with equality holds if and only if \( G \) is bipartite. This is why the weighted vertex PI index was introduced. If \( G \) is a bipartite graph, then

\[
PL_w(G) = n \sum_{u \in V(G)} d^2(u).
\]

A graph is a cactus if it is connected and all its blocks are either edges or cycles, i.e. any two of its cycles have at most one common vertex. Up to now, many results were obtained concerning the cacti between chemistry and graph theory. Chen [2] gave the first three smallest Gutman indices among the cacti. Feng and Yu [8] established the cacti with the smallest hyper-Wiener indices. Li et al. [24] determined sharp upper and lower bounds of the cacti for Zagreb indices. Wang and Kang [38] found the bounds of Harary index for the cacti. Wang and Tan [39] characterized the extremal cacti having the largest Wiener and hyper-Wiener indices. In [40], Wang et al. determine the extremal graphs with greatest and smallest vertex PI index among all cacti with a fixed number of vertices and pendant vertices.

Motivated by the results of chemical indices and their applications, it may be interesting to characterize the cacti with greatest and smallest weighted vertex PI indices.

Denote by \( C: A(n, s) \) the set of cacti of order \( n \) and with \( s \) cycles. Let \( S_n \) be the star of order \( n \). Denote by \( S^*_n \) the graph obtained by inserting one new edge between the leaves of the star \( S_n \). Let \( S^{*1}_{n,s} \) be the graph of order \( n \) obtained by inserting \( s \) independent new edges between the leaves of a star \( S_n \), see Figure 1. In particular, \( S^*_n \) is just \( S^{*1}_{n,1} \).
Figure 1: The graph $S^s_n$. It has $s$ triangles and $n - 2s - 1$ pendent edges.

In the following theorem, among all the graphs in $\mathcal{CA}(n,s)$, the upper bound on the weighted vertex PI index and the corresponding extremal graph are given.

**Theorem 1.1.** For any graph $G \in \mathcal{CA}(n,s)$ where $n \geq 2s + 1$,

$$PI_w(G) \leq n^3 - n^2 + 6s$$

with the equality holds if and only if $G \cong S^s_n$.

Let $\mathcal{T}(n,s)$ be the set of graphs such that $\mathcal{T}(n,s) \subset \mathcal{CA}(n,s)$ and for any graph $G \in \mathcal{T}(n,s)$, it satisfy the following four conditions: (1) for any vertex $v \in V(G)$, $d_G(v) \in \{2, 3\}$; (2) if $d_G(v) = 3$ for some vertex $v \in V(G)$, $v$ should be in some cycle of $G$; (3) all cycles of $G$ are of odd length; (4) for a cycle $C$ in $G$, if there are two or more 3-vertices in $C$, the cycle $C$ is a 3-cycle. See Figure 2.

Figure 2: Three graphs in $\mathcal{T}(14,4)$.

In the following theorem, among all the graphs in $\mathcal{CA}(n,s)$, the lower bound on the weighted vertex PI index and the corresponding extremal graph are given.

**Theorem 1.2.** For any graph $G \in \mathcal{CA}(n,s)$ where $n \geq 3s$,

$$PI_w(G) \geq 4n^2 + (5s - 8)n - s - 2$$

with the equality holds if and only if $G \in \mathcal{T}(n,s)$.

For any cut edge $e = uv$ of a connected graph $G$ where $|G| = n$, $n_u(e|G) + n_v(e|G) = n$. So the following lemma, which is similar to the corresponding property of matching energy [12], can be got.
Lemma 1.3. Suppose that G is a connected graph and T an induced subgraph of G such that T is a tree and T is connected to the rest of G only by a cut vertex v. If T is replaced by a star of the same order, centered at v, then the weighted vertex PI index of G increases (unless T is already such a star). If T is replaced by a path of the same order, with one end at v, then the weighted vertex PI index of G decreases (unless T is already such a path).

In Section 2, Theorem 1.1 is proved. In Section 3, Theorem 1.2 is proved.

2. The upper bound

In this section, the upper bound on the weighted vertex PI index of the graphs in $CA(n, s)$ and the corresponding extremal graphs are given, that is, Theorem 1.1 is proved.

![Figure 3: PLω(G1) < PLω(G2) < PLω(G3).](image)

Lemma 2.1. Suppose that $H_1$ and $H_2$ are two graphs with $v_i \in V(H_i)$ for $i = 1, 2$. Suppose $P_n, T_n, S_n$ are path, tree and star of the same order $n$ such that $T_n \neq P_n$ and $T_n \neq S_n$. Let $G_1$ be the graph obtained by identifying the vertex $v_1$ with one end of $P_n$ and identifying the vertex $v_2$ with the other end of $P_n$. Let $G_2$ be the graph obtained by identifying the vertex $v_1$ with one vertex of $T_n$ and identifying the vertex $v_2$ with another vertex of $T_n$. Let $G_3$ be the graph obtained by identifying the vertex $v_1$ and $v_2$ as a new vertex $v$, and then identifying the vertex $v$ with the center of $S_n$. See Figure 3. Then we have

$$PL_\omega(G_1) < PL_\omega(G_2) < PL_\omega(G_3).$$

Proof. Because $T_n \neq P_n$ and $T_n \neq S_n$, $n \geq 4$.

For any edge $e = v_1v'_1 \in E(H_1)$, $n_v(e|G_1) + n_{v'_1}(e|G_1) = n_v(e|G_2) + n_{v'_1}(e|G_2) = n_v(e|G_3) + n_{v'_1}(e|G_3)$ and $d_G(v_1) + d_G(v'_1) \leq d_{G_2}(v_1) + d_{G_2}(v'_1) < d_{G_3}(v_1) + d_{G_3}(v'_1)$. So

$$\sum_{e=v_1v'_1 \in E(H_1)} (d_G(v_1) + d_G(v'_1))(n_v(e|G_1) + n_{v'_1}(e|G_1)) \leq \sum_{e=v_1v'_1 \in E(H_1)} (d_{G_2}(v_1) + d_{G_2}(v'_1))(n_v(e|G_2) + n_{v'_1}(e|G_2)) < \sum_{e=v_1v'_1 \in E(H_1)} (d_{G_3}(v_1) + d_{G_3}(v'_1))(n_v(e|G_3) + n_{v'_1}(e|G_3)).$$

Similarly, for any edge $e = v_2v'_2 \in E(H_2)$, $n_v(e|G_1) + n_{v'_2}(e|G_1) = n_v(e|G_2) + n_{v'_2}(e|G_2) = n_v(e|G_3) + n_{v'_2}(e|G_3)$ and $d_G(v_2) + d_G(v'_2) \leq d_{G_2}(v_2) + d_{G_2}(v'_2) < d_{G_3}(v_2) + d_{G_3}(v'_2)$. So

$$\sum_{e=v_2v'_2 \in E(H_2)} (d_G(v_2) + d_G(v'_2))(n_v(e|G_1) + n_{v'_2}(e|G_1)) \leq \sum_{e=v_2v'_2 \in E(H_2)} (d_{G_2}(v_2) + d_{G_2}(v'_2))(n_v(e|G_2) + n_{v'_2}(e|G_2)) < \sum_{e=v_2v'_2 \in E(H_2)} (d_{G_3}(v_2) + d_{G_3}(v'_2))(n_v(e|G_3) + n_{v'_2}(e|G_3)).$$
For any edge $e = xy \in E(P_n)$, $n_x(e|G_1) + n_y(e|G_1) = |G_1|$. Similarly, for any edge $e = xy \in E(T_n)$, $n_x(e|G_2) + n_y(e|G_2) = |G_2|$, and for any edge $e = xy \in E(S_n), n_x(e|G_3) + n_y(e|G_3) = |G_3|$. Note that $|G_1| = |G_2| = |G_3|$. So

$$\sum_{e=xy \in E(P_n)} (d_{G_1}(x) + d_{G_1}(y))(n_x(e|G_1) + n_y(e|G_1)) < \sum_{e=xy \in E(T_n)} (d_{G_2}(x) + d_{G_2}(y))(n_x(e|G_2) + n_y(e|G_2))$$

$$< \sum_{e=xy \in E(S_n)} (d_{G_3}(x) + d_{G_3}(y))(n_x(e|G_3) + n_y(e|G_3)).$$

It is now straightforward to show that $PL_w(G_1) - PL_w(G_2) < 0$.

Similarly, we can prove $PL_w(G_2) < PL_w(G_3)$. The proof completes. $\square$

Lemma 2.2. Suppose that $H$ is a graph with $v \in V(H)$ and $C_r$ is a cycle of order $r$. Let $H(v)C_r$ be the graph obtained by identifying the vertex $v$ with one vertex of $C_r$. Let $G_3$ be the graph obtained from $H(v)C_r$ by attaching at vertices of $C_r$ except $v$ some pendent edges. Let $G_2$ be the graph obtained from $G_3$ by moving all pendent edges, which are rooted on vertices of $C_r$ except $v$, on $v$. Note that $|G_1| = |G_2|$. See Figure 4. Then we have

$$PL_w(G_1) < PL_w(G_2).$$

Proof. Suppose $|G_1| = |G_2| = n$. In $G_1$ and $G_2$, suppose the vertices of $C_r$ are $v_0(v)v_1v_2\cdots v_{r-1}$ subsequently. In $G_1$, suppose there are $t_i$ pendent edges rooted on $v_i$ for $1 \leq i \leq r - 1$ and $\sum_{i=1}^{r-1} t_i = t$.

Note that $d_{G_1}(v) = d_{G_1}(v) - t$. For any edge $e = vv' \in E(H)$, $d_{G_1}(v) + d_{G_1}(v') < d_{G_1}(v) + d_{G_1}(v')$ and $n_x(e|G_1) + n_{x'}(e|G_1) = n_x(e|G_2) + n_{x'}(e|G_2)$. So

$$\sum_{e=vv' \in E(H)} (d_{G_1}(v) + d_{G_1}(v'))(n_x(e|G_1) + n_{x'}(e|G_1)) - \sum_{e=vv' \in E(H)} (d_{G_2}(v) + d_{G_2}(v'))(n_x(e|G_2) + n_{x'}(e|G_2))$$

$$< 0.$$

In $G_1$, for the pendent edge $e = v_iv_i'$ rooted on $v_i$ (1 \leq i \leq r - 1), d_{G_1}(v_i) + d_{G_1}(v_i') = t_i + 2 + 1 = t_i + 3$ and $n_x(e|G_1) + n_{x'}(e|G_1) = n$.

$$\sum_{i=1}^{r-1} \sum_{e=vv' \in E(G_1)} (d_{G_1}(v_i) + d_{G_1}(v_i'))(n_x(e|G_1) + n_{x'}(e|G_1)) = n \sum_{i=1}^{r-1} t_i(t_i + 3)$$

Figure 4: $PL_w(G_1) < PL_w(G_2)$. 

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In $G_2$, for the pendent edge $e = vv'$ which is not in $E(H)$ and rooted on $v$, $d_{G_2}(v) + d_{G_2}(v') = d_{G_1}(v) + t + 1$ and $n_{e}(e|G_2) + n_{e'}(e|G_2) = n$.

$$\sum_{e=e'=E(G_2)\setminus E(H), d_{G_2}(e')=1}(d_{G_1}(v) + d_{G_1}(v'))(n_{e}(e|G_2) + n_{e'}(e|G_2)) = tn(d_{G_1}(v) + t + 1).$$

First suppose $r$ is even. For the edge $e = v_iv_{i+1}$ $(0 \leq i \leq r - 1)$ of $C$, in $G_1$, $d_{G_1}(v_i) + d_{G_1}(v_{i+1}) = t_i + t_{i+1} + 4$ when $1 \leq i \leq r - 2$, $d_{G_1}(v_0) + d_{G_1}(v_1) = d_{G_1}(v) + t_1 + 2$ when $i = 0$ and $d_{G_1}(v_{r-1}) + d_{G_1}(v_0) = d_{G_1}(v) + t_{r-1} + 2$ when $i = r - 1$. Because $r$ is even, $n_{v}(e|G_1) + n_{v_{r+1}}(e|G_1) = n$.

$$\sum_{i=0}^{r-1}(d_{G_1}(v_i) + d_{G_1}(v_{i+1}))(n_{v_i}(e|G_1) + n_{v_{i+1}}(e|G_1))$$
$$= 2n(d_{G_1}(v) + t + 2(r - 1)).$$

For the edge $e = v_iv_{i+1}$ $(0 \leq i \leq r - 1)$ of $C$ in $G_2$, $d_{G_2}(v_i) + d_{G_2}(v_{i+1}) = 4$ when $1 \leq i \leq r - 2$, $d_{G_2}(v_0) + d_{G_2}(v_1) = d_{G_2}(v) + 2$ when $i = 0$ and $d_{G_2}(v_{r-1}) + d_{G_2}(v_0) = d_{G_2}(v) + 2$ when $i = r - 1$. Because $r$ is even, $n_{v}(e|G_2) + n_{v_{r+1}}(e|G_2) = n$.

$$\sum_{i=0}^{r-1}(d_{G_1}(v_i) + d_{G_1}(v_{i+1}))(n_{v_i}(e|G_2) + n_{v_{i+1}}(e|G_2))$$
$$= 2n(d_{G_1}(v) + 2(r - 1))$$
$$= 2n(d_{G_1}(v) + t + 2(r - 1)).$$

Now we are ready to compare $P_{I_v}(G_1)$ with $P_{I_v}(G_2)$.

$$P_{I_v}(G_1) - P_{I_v}(G_2) = \sum_{e=e'=E(H)}(d_{G_1}(v) + d_{G_1}(v'))(n_{e}(e|G_1) + n_{e'}(e|G_1))$$
$$+ \sum_{i=1}^{r-1}\sum_{e=e'=E(G_1)}(d_{G_1}(v_i) + d_{G_1}(v_{i+1}))(n_{v_i}(e|G_1) + n_{v_{i+1}}(e|G_1))$$
$$+ \sum_{i=0}^{r-1}(d_{G_1}(v_i) + d_{G_1}(v_{i+1}))(n_{v_i}(e|G_1) + n_{v_{i+1}}(e|G_1))$$
$$- \sum_{e=e'=E(H)}(d_{G_2}(v) + d_{G_2}(v'))(n_{e}(e|G_2) + n_{e'}(e|G_2))$$
$$- \sum_{e=e'=E(G_2)\setminus E(H), d_{G_2}(e')=1}(d_{G_2}(v) + d_{G_2}(v'))(n_{e}(e|G_2) + n_{e'}(e|G_2))$$
$$- \sum_{i=0}^{r-1}(d_{G_2}(v_i) + d_{G_2}(v_{i+1}))(n_{v_i}(e|G_2) + n_{v_{i+1}}(e|G_2))$$
$$< 0.$$

When $r$ is odd, $P_{I_v}(G_1) < P_{I_v}(G_2)$ can be proved similarly since the only difference being that

$$n_{v}(e|G_1) + n_{v_{r+1}}(e|G_1) = n_{v}(e|G_2) + n_{v_{r+1}}(e|G_2) = n - 1.$$

The proof completes. □
Lemma 2.3. Suppose that \( H \) is a graph with \( v \in V(H) \) where \( d_H(v) \geq 2 \) and \( C_r \) is a cycle of order \( r \) where \( r \geq 4 \). Let \( G_1 = H(v)C_r \), be the graph obtained by identifying the vertex \( v \) with one vertex of \( C_r \). Let \( G_2 \) be the graph obtained from \( G_1 \) by replacing \( C_r \) by \( C_3 \) and \( r - 3 \) pendent edges. Note that \(|G_1| = |G_2| \). See Figure 5. Then we have

\[ PL_w(G_1) < PL_w(G_2). \]

Proof. Suppose \(|G_1| = |G_2| = n\) without of generality. Note that \( d_{G_2}(v) = d_{G_1}(v) - (r - 3) \). For any edge \( e = vv' \in E(H) \), \( d_{G_1}(v) + d_{G_1}(v') < d_{G_2}(v) + d_{G_2}(v') \) and \( n_{e}(e|G_1)) + n_{e'}(e|G_1)) = n_{e}(e|G_2) + n_{e'}(e|G_2) \). So

\[ \sum_{e = vv' \in E(H)} (d_{G_1}(v) + d_{G_1}(v'))(n_{e}(e|G_1)) + n_{e'}(e|G_1)) \]

\[ - \sum_{e = vv' \in E(H)} (d_{G_2}(v) + d_{G_2}(v'))(n_{e}(e|G_2)) + n_{e'}(e|G_2)) \]

\[ < 0. \]

When \( r \) is odd, for the edges in \( C_r \) of \( G_1 \),

\[ \sum_{i=0}^{r-1} (d_{G_1}(v_i) + d_{G_1}(v_{i+1}))(n_{e}(e|G_1)) + n_{e'}(e|G_1)) \]

\[ = 4(r - 1) + (n - 1)[2(d_{G_1}(v) + 2) + 4(r - 3)]. \]

When \( r \) is even, for the edges in \( C_r \) of \( G_1 \),

\[ \sum_{i=0}^{r-1} (d_{G_1}(v_i) + d_{G_1}(v_{i+1}))(n_{e}(e|G_1)) + n_{e'}(e|G_1)) \]

\[ = n[2(d_{G_1}(v) + 2) + 4(r - 2)]. \]

For any pendent edge \( vv' \) rooted on \( v \) in \( G_2 \), \( d_{G_2}(v) + d_{G_2}(v') = d_{G_1}(v) + 1 = d_{G_1}(v) + r - 2 \) and \( n_{e}(e|G_2) + n_{e'}(e|G_2) = n \). So

\[ \sum_{e = vv' \in E(G_2) \setminus E(H), d_{G_2}(v') = 1} (d_{G_2}(v) + d_{G_2}(v'))(n_{e}(e|G_2)) + n_{e'}(e|G_2)) = (r - 3)n(d_{G_1}(v) + r - 2). \]

For the edges in \( C_3 \) of \( G_2 \),

\[ \sum_{i=0}^{2} (d_{G_1}(v_i) + d_{G_1}(v_{i+1}))(n_{e}(e|G_2)) + n_{e'}(e|G_2)) \]

\[ = 4 \times 2 + 2(d_{G_1}(v) + 2)(n - 1) \]

\[ = 8 + 2(d_{G_1}(v) + r - 1)(n - 1). \]
It is now straightforward to show that $PI_w(G_2) - PI_w(G_1) > 0$. The proof completes.

### Lemma 2.4

Suppose that $H$ is a graph with $v \in V(H)$ and $C_r$ is a cycle of order $r$. Let $H(v)C_r$ be the graph obtained by identifying the vertex $v$ with one vertex of $C_r$. Let $G_1$ be the graph obtained from $H(v)C_r$ by attaching at vertices of $C_r$ except $v$ some triangles and (or) some pendent edges. Let $G_2$ be the graph obtained from $G_1$ by moving all triangles and pendent edges, which are rooted on vertices of $C_r$ except $v$, on $v$. Note that $|G_1| = |G_2|$. See Figure 6. Then we have

$$PI_w(G_1) < PI_w(G_2).$$

We leave to the reader the proof of Lemma 2.4, since it is similar to the proof of Lemma 2.2.

Now we are ready to give the proof of Theorem 1.1.

**Proof.** [Proof of Theorem 1.1] Via Lemma 1.3, Lemma 2.1, Lemma 2.2, Lemma 2.3 and Lemma 2.4, for any graph $G \in CA(n, s)$, $PI_w(G) \leq PI_w(S_{r+1}^n)$ and the equality holds if and only if $G \cong S_{r+1}^n$.

It is easy to compute that $PI_w(S_{r+1}^n) = n^3 - n^2 + 6s$. The proof completes.

### 3. The lower bound

In this section the lower bound on the weighted vertex PI index of the graphs in $CA(n, s)$ and the corresponding extremal graphs are given, that is, Theorem 1.2 is proved.

**Lemma 3.1** Suppose that $H$ is a graph with $u \in V(H)$ and $C_r$ is a cycle of order $r$ with $v \in V(C_r)$. Let $H(u)P_{s+1}(v)C_r$ be the graph obtained by identifying the vertex $u$ with one end of $P_{s+1}$ and identifying the vertex $v$ with the other end of $P_{s+1}$. Let $G_1$ be the graph obtained from $H(u)P_{s+1}(v)C_r$ by attaching at vertices of $C_r$ except $v$ some paths, and the
total length of these paths is \( t \) with \( t \geq 1 \). Let \( G_2 = H(u)P_{s+1}(v)C_r \). Note that \( |G_1| = |G_2| \). See Figure 7. Then we have

\[
\text{Pl}_w(G_1) > \text{Pl}_w(G_2).
\]

Proof. Suppose \( |G_1| = |G_2| = n \). Denote the vertices of \( C_r \) by \( v_0, v_1, v_2, \ldots, v_{r-1} \) subsequently. For simplicity, suppose that \( s \geq 1 \) and there is a path of length \( t_i \) rooted on \( v_i \) (\( 1 \leq i \leq r - 1 \)) where \( t_i \geq 1 \) and \( \sum_{i=1}^{r-1} t_i = t \).

In \( G_1 \), we consider the edges in the paths rooted on \( v_i \) (\( 1 \leq i \leq r - 1 \)) and the edges in \( C_r \) subsequently. In \( G_2 \), we consider the \( t \) new added edges in the path connecting \( H \) and \( C_r \), and the edges in \( C_r \) subsequently. When \( r \) is odd,

\[
\text{Pl}_w(G_1) - \text{Pl}_w(G_2) = 4tn + \sum_{i=0}^{r-1} (d_{G_1}(v_i) + d_{G_1}(v_{i+1}))(n_{e,1}(e|G_1) + n_{e,2}(e|G_1))
\]

\[
- 4tn - \sum_{j=0}^{r-1} (d_{G_2}(v_j) + d_{G_2}(v_{j+1}))(n_{e,2}(e|G_2) + n_{e,3}(e|G_2))
\]

\[
= 6t \sum_{i=1}^{r-1} (t_i + 1) + \sum_{i=1}^{r-1} (n - t_i - 1)] - [4(r - 1) + (n - 1)(5 \times 2 + 4(r - 3))] - 4(r - 3)n
\]

\[
> 0.
\]

When \( r \) is even, \( \text{Pl}_w(G_1) > \text{Pl}_w(G_2) \) can be proved similarly. This completes the proof.

![Figure 8: Pl_w(G_1) ≥ Pl_w(G_2). The equality holds if and only if r is odd.](image)

**Lemma 3.2.** Suppose that \( H \) is a graph with \( u \in V(H) \) where \( d_H(u) \geq 2 \) and \( C_r \) is a cycle of order \( r \) where \( r \geq 4 \). Let \( G_1 \) be the graph such that one end of a path \( P_{s+1} \) is connected with \( u \) of \( H \) and the other end of \( P_{s+1} \) is connected with one vertex of \( C_r \). Let \( G_2 \) be the graph such that one end of a path \( P_{s+r-2} \) is connected with \( u \) of \( H \) and the other end of \( P_{s+r-2} \) is connected with one vertex of \( C_3 \). Note that \( |G_1| = |G_2| \). See Figure 8. Then we have

\[
\text{Pl}_w(G_1) \geq \text{Pl}_w(G_2),
\]

with the equality holds if and only if \( s \geq 1 \) and \( r \) is odd.

Proof. Suppose \( |G_1| = |G_2| = n \). Denote the vertices of \( C_r \) in \( G_1 \) by \( v_0(v), v_1, v_2, \ldots, v_{r-1} \) subsequently. Denote the vertices of \( C_3 \) in \( G_2 \) by \( v_0(v), v_1, v_2 \) subsequently.

First suppose \( s \geq 1 \). In \( G_1 \), we consider the edges in \( C_r \). In \( G_2 \), we consider the new added \( r - 3 \) edges in the path connecting \( H \) and \( C_3 \), and the edges in \( C_3 \) subsequently.

\[
\text{Pl}_w(G_1) - \text{Pl}_w(G_2) = \sum_{i=0}^{r-1} (d_{G_1}(v_i) + d_{G_1}(v_{i+1}))(n_{e,1}(e|G_1) + n_{e,2}(e|G_1))
\]

\[
- 4(r - 3)n - \sum_{i=0}^{2} (d_{G_2}(v_i) + d_{G_2}(v_{i+1}))(n_{e,2}(e|G_2) + n_{e,3}(e|G_2)).
\]
When $r$ is even,
\[
PL_w(G_1) - PL_w(G_2) = [2 \times 5 + 4(r-2)]n - 4(r-3)n - 2 \times 5(n-1) - 4 \times 2.
\]
When $r$ is odd,
\[
PL_w(G_1) - PL_w(G_2) = [2 \times 5 + 4(r-3)](n-1) + 4(r-1) - 4(r-3)n - 2 \times 5(n-1) - 4 \times 2 - n(n-1).
\]
When $s = 0$, $H$ and $C_r$ share a common vertex $u$. $PL_w(G_1) > PL_w(G_2)$ can be proved similarly in this case. The proof completes.

\[
\text{Figure 9: } PL_w(G_1) > PL_w(G_2).
\]

**Lemma 3.3.** Let $C_r$ be a cycle with $r \geq 4$ and $u_0, u_1, \ldots, u_{r-1}$ are the vertices of $C_r$ subsequently. Let $H_0$ be a cactus graph such that $|H_0| \geq 2$ and all edges in $H_0$ are triangles. Suppose $v, x$ are two vertices of $V(H_0)$ such that $v, x$ are in some triangles of $H_0$ and $d_{H_0}(v) = d_{H_0}(x) = 2$. Let $G_1$ be the graph obtained by connecting $u_0$ and $v$ via a path (the length of the path $\geq 0$), and identifying $u_i$, where $i \neq 0$ with one vertex of a graph $H$. Let $G_2$ be the graph obtained from $G_1$ by deleting the edge $u_iw$ for any $w \in V(H)$ and adding the edge $xw$. See Figure 9. Then we have

\[
PL_w(G_1) > PL_w(G_2).
\]

**Proof.** Suppose $|G_1| = |G_2| = n$. In $G_1$, suppose $1 < i < r - 1$ and the other vertices of $C_r$ except $u_0, u_i$ are of degree $2$ for simplicity. Suppose $H_0$ be a triangle for simplicity and $v, x, y$ are the three vertices of $H_0$. Suppose the path connecting $u_0$ and $v$ is of length $\geq 1$ for simplicity. Note that $d_{G_i}(u_i) = d_{G_i}(x)$.

Suppose the number of vertices which are equidistant with $v, y$ in $G_2$ is $t_1$ and the number of vertices which are equidistant with $x, y$ in $G_2$ is $t_2$. Note that $t_1 = |H|$ and $t_1 + t_2 = n - 1$.

When $r$ is even, we consider the edges $u_iu_{i-1}, u_iu_{i+1}, vx, vy, xy$ respectively.

\[
PL_w(G_1) - PL_w(G_2) = 2n[(d_{G_i}(u_i) + 2)] + 5(n-1) + 5(n-1) + 4 \times 2
\]
\[= [2n(2 + 2) + (d_{G_i}(x) + 3)(n-1) + 5(n-t_1) + (d_{G_i}(x) + 2)(n-t_2)]
\]
\[= 2nd_{G_i}(u_i) + 14n - 2 - [2nd_{G_i}(x) + 13n - d_{G_i}(x) + 2 - (d_{G_i}(x) - 3)t_2]
\]
\[= n + d_{G_i}(x) + (d_{G_i}(x) - 3)t_2 - 4 > 0.
\]

When $r$ is odd and $i \notin \left[\frac{r-1}{2}, \frac{r+1}{2}\right]$, we consider the edges $u_iu_{i-1}, u_iu_{i+1}, u_{\frac{r+1}{2} \times 2}, u_{\frac{r}{2} \times 2}$, the edge in $C_r$ whose two
vertices have the same distance to $u_i, vx, vy, xy$ respectively.

$$PI_w(G_1) - PI_w(G_2)$$
$$= 2[d_{G_1}(u_i) + 2|(n - 1) + 4(n - 4) + 4(n - |H|) + 5(n - 1) + 5(n - 1) + 4 \times 2$$
$$- [2 \times 4(n - 1) + 4(n - |H| - 3) + 4(n - 1) + (d_{G_1}(x) + 3)(n - 1) + 5(n - t_1)$$
$$+ (d_{G_1}(x) + 2)(n - t_2)]$$
$$= 2nd_{G_1}(u_i) + 14n - 2d_{G_1}(u_i) - 6 - [2nd_{G_1}(x) + 13n - d_{G_1}(x) - 6 - (d_{G_1}(x) - 3)t_2]$$
$$= n - d_{G_1}(x) + (d_{G_1}(x) - 3)t_2$$
$$> 0.$$

When $r$ is odd and $i \in \{\frac{n+1}{2}, \frac{n+3}{2}\}$, suppose $i = \frac{n+1}{2}$. We consider the edges $u_iu_j, u_iu_{j+1}, u_0u_{r-1}, vx, vy, xy$ respectively. Note that $n - t_2 = |H| + 1$.

$$PI_w(G_1) - PI_w(G_2)$$
$$= [d_{G_1}(u_i) + 2|(n - 1) + [d_{G_1}(u_i) + 2|(n - 4) + 5(n - |H|) + 5(n - 1) + 5(n - 1) + 4 \times 2$$
$$- [4(n - 1) + 4(n - |H| - 3) + 5(n - 1) + (d_{G_1}(x) + 3)(n - 1) + 5(n - t_1)$$
$$+ (d_{G_1}(x) + 2)(n - t_2)]$$
$$= n - |H| + 7 + (t_2 - 4)d_{G_1}(x) - 3t_2$$
$$> 0.$$

The last inequality holds since $t_2 > 4$. The proof completes. □

In Lemma 3.3, for the cycle $C_r$ in $G_1$ or $G_2$, if there is a graph connecting with $C_r$ via $u_j$ ($1 \leq j \leq r - 1$ and $j \neq i$) where $u_j$ is a cut vertex, the conclusion is still correct.

![Figure 10: $PI_w(G_1) \geq PI_w(G_2)$](image)

The equality holds if and only if $r = 3$.

Now we are ready to give the proof of Theorem 1.2.

**Proof.** [Proof of Theorem 1.2] Let $G \in C_\mathcal{A}(n, s)$. From Lemma 2.1, Lemma 3.1, Lemma 3.2 and Lemma 3.3, we can assume that $\delta(G) \geq 2$ and all cycles of $G$ are triangles. If $G \in T(n, s)$, nothing needs to be proved. If $G \notin T(n, s)$, $G$ can be dealt with via the following transformations:
(1) If there are two triangles share a common vertex in $G$, borrow an edge from other place of $G$ and then insert the edge between the two triangles. See (a) of Figure 10.

(2) If there are $t$ ($t \geq 3$) triangles share a common vertex in $G$, move one triangle to a 2-vertex of one triangle and then repeat the above step $t - 3$ times. Now for any vertex which is shared by two triangles, repeat (1). See (b) of Figure 10.

(3) If there is a $t$-vertex ($t \geq 3$) in $G$ which is not in any triangle, move the first edge, which is adjacent to the above vertex, to a 2-vertex of one triangle and then repeat the above step $t - 3$ times. See (c) of Figure 10.

Other cases not mentioned can be dealt with similarly.

It is easy to see that $PI_w(G)$ decreases after the above transformations and $G \in \mathcal{T}(n, s)$ at last.

For any graph $G \in \mathcal{T}(n, s)$, It is easy to compute that $PI_w(G) = 4n^2 + (5s - 8)n + s - 2$. The proof completes. □

References

[1] J. A. Bondy, U. S. R. Murty, Graph Theory. Springer, Berlin, 2008.
[2] S. Chen, Cacti with the smallest, second smallest and third smallest Gutman index. J. Comb. Optim. 31(2016)327-332.
[3] K. C. Das, I. Gutman, Bound for vertex PI index in terms of simple graph parameters. Filomat, 27(2013)1583-1587.
[4] H. Deng, A unified approach to the extremal Zagreb indices for trees, unicyclic graphs and bicyclic graph. MATCH Commun. Math. Comput. Chem. 57(2007)597-616.
[5] P. V. Khadikar, S. Karmarkar, V. K. Agrawal, A novel PI index and its applications to QSPR/QSAR studies. J. Chem. Inf. Comput. Sci. 41(2001)934-949.
[6] M. H. Khalifeh, H. Yousefi-Azari, A. R. Ashrafi, Vertex and edge PI indices of Cartesian product graphs. Disc. Appl. Math. 156(2008)1780-1789.
[7] M. H. Khalifeh, H. Yousefi-Azari, A. R. Ashrafi, A matrix method for computing Szeged and vertex PI indices of join and composition of graphs. Linear Algebra. Appl. 429(2008)2702-2709.
[8] M. H. Khalifeh, H. Yousefi-Azari, A. R. Ashrafi, Order of Magnitude of the PI index. MATCH Commun. Math. Comput. Chem. 65(2011)51-56.
[9] G. Ma, Q. Bian, J. Wang, Bounds on the PI index of unicyclic and bicyclic graphs with given girth. Disc. Appl. Math. 230(2017)156-161.
[10] K. Pattabiraman, P. Kandan, Wiener PI index of corona product of graphs. Disc. Math. Algorith. Appl. 6(4)(2014)1450055 (9pages).
[11] K. Pattabiraman, P. Kandan, On weighted PI index of graphs. Electro. Notes Disc. Math. 53(2016)223-238.
[12] K. Pattabiraman, P. Paulraja, Wiener and vertex PI indices of the strong product of graphs. Discuss. Math. Graph Theory, 32(2012)749-769.
[37] Ž. K. Vukičević, D. Stevanović, Bicyclic graphs with extremal values of PI index. *Disc. Appl. Math.* 161(2013)395-403.
[38] H. Wang, L. Kang, On the Harary index of cacti, *Util. Math.* 96(2015)149-163.
[39] D. Wang, S. Tan, The maximum hyper-Wiener index of cacti, *J. Appl. Math. Comput.* 47(2015)91-102.
[40] C. Wang, S. Wang, B. Wei, Cacti with extremal PI index. *Transactions on Combin.* 5(4)(2016)1-8.
[41] H. Wiener, Structural determination of the paraffin boiling points. *J. Am. Chem. Soc.* 69(1947)17-20
[42] F. Xia, S. Chen, Ordering unicyclic graphs with respect to Zagreb indices. *MATCH Commun. Math. Comput. Chem.* 58(2007)663-673.
[43] L. You, R. Zhu, Z. You, The (weighted) vertex PI index of unicyclic graphs. *MATCH Commun. Math. Comput. Chem.* 67(2012)383-404.
[44] H. Yousefi-Azari, B. Manoochehrian, A. R. Ashrafi, The PI index of product graphs. *Appl. Math. Lett.* 21(2008)624-627.