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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

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

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

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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

$$PI_v(G) = \sum_{e=uv\in E(G)} [n_u(e|G) + n_v(e|G)].$$

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:

$$M_1(G) = \sum_{u\in V(G)} d_G^2(u),$$

where $d_G(u)$ 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:

$$PI_w(G) = \sum_{e=uv\in E(G)} (d_G(u) + d_G(v))(n_u(e|G) + n_v(e|G)).$$

For any edge e of a bipartite graph, $n_u(e|G) + n_v(e|G) = n$. Therefore the diversity of the vertex PI index is not satisfying for bipartite graphs. The inequality $PI_v(G) \leq n \cdot m$ holds 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

$$PI_w(G) = n \sum_{u\in V(G)} d_G^2(u).$$

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, $PI_w(G) \geq n(4n-6)$, with equality holds if and only if $G \cong P_n$, and $PI_w(G) \leq \frac{8}{27}n^4$, with equality holds if and only if $3|n$ and $G \cong K_{\frac{n}{3},\frac{n}{3},\frac{n}{3}}$. In the same paper, the exact expressions for the weighted vertex PI index of the Cartesian product of graphs are also given. In [43] and [28], bounds and the extremal graphs on the weighted vertex PI index of connected unicyclic and bicyclic graph are given respectively. In [34], the exact formula for the weighted vertex PI index of corona product of two connected graphs is obtained. In [35], the exact formulas for the weighted vertex PI index of generalized hierarchical product and join of two graphs are obtained. In [29], the weighted vertex PI index of (n,m)-graphs with given diameter was studied.

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 pendent 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 $\mathcal{CA}(n,s)$ 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 $S_n^{+,s}$ 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 $S_n^{+,1}$.

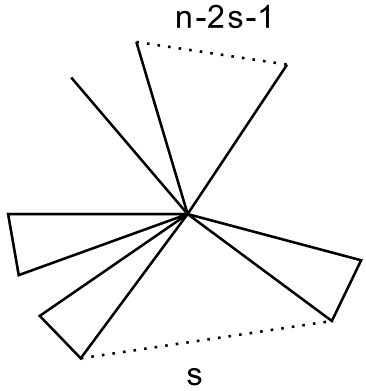

Figure 1: The graph $S_n^{+,s}$. It has s triangles and $n-2s-1$ pendent edges.

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 $G \cong S_n^{+,s}$.

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.

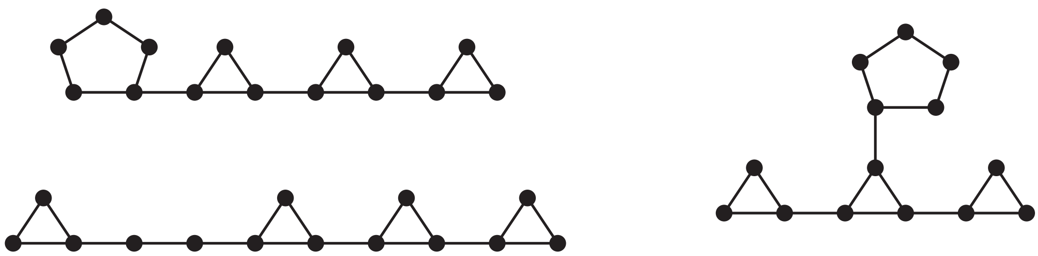

Figure 2: Three graphs in $\mathcal{T}(14,4)$.

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 $\mathcal{CA}(n,s)$ and the corresponding extremal graphs are given, that is, Theorem 1.1 is proved.

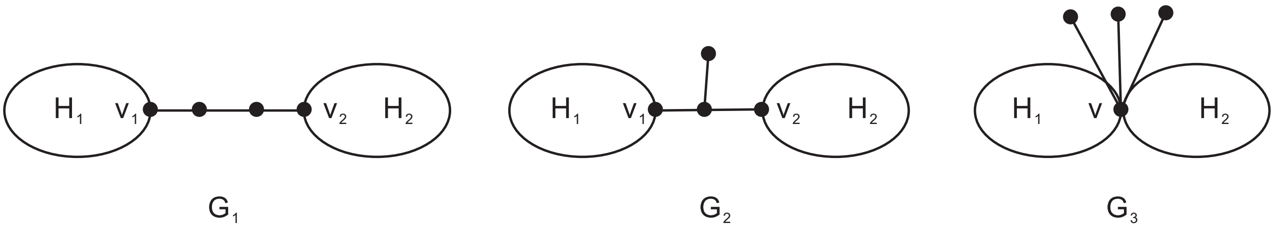

Figure 3: $PI_w(G_1) < PI_w(G_2) < PI_w(G_3)$.

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 $T_n \ncong P_n$ and $T_n \ncong S_n$. 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*

$$PI_w(G_1) < PI_w(G_2) < PI_w(G_3).$$

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

For any edge $e = v_1v_1' \in E(H_1)$, $n_{v_1}(e|G_1) + n_{v_1'}(e|G_1) = n_{v_1}(e|G_2) + n_{v_1'}(e|G_2) = n_{v_1}(e|G_3) + n_{v_1'}(e|G_3)$ and $d_{G_1}(v_1) + d_{G_1}(v_1') \leq d_{G_2}(v_1) + d_{G_2}(v_1') < d_{G_3}(v_1) + d_{G_3}(v_1')$. So

$$\begin{aligned}
&\sum_{e=v_1v_1'\in E(H_1)} (d_{G_1}(v_1) + d_{G_1}(v_1'))(n_{v_1}(e|G_1) + n_{v_1'}(e|G_1)) \\
\leq &\sum_{e=v_1v_1'\in E(H_1)} (d_{G_2}(v_1) + d_{G_2}(v_1'))(n_{v_1}(e|G_2) + n_{v_1'}(e|G_2)) \\
< &\sum_{e=v_1v_1'\in E(H_1)} (d_{G_3}(v_1) + d_{G_3}(v_1'))(n_{v_1}(e|G_3) + n_{v_1'}(e|G_3)).
\end{aligned}$$

Similarly, for any edge $e = v_2v_2' \in E(H_2)$, $n_{v_2}(e|G_1) + n_{v_2'}(e|G_1) = n_{v_2}(e|G_2) + n_{v_2'}(e|G_2) = n_{v_2}(e|G_3) + n_{v_2'}(e|G_3)$ and $d_{G_1}(v_2) + d_{G_1}(v_2') \leq d_{G_2}(v_2) + d_{G_2}(v_2') < d_{G_3}(v_2) + d_{G_3}(v_2')$. So

$$\begin{aligned}
&\sum_{e=v_2v_2'\in E(H_2)} (d_{G_1}(v_2) + d_{G_1}(v_2'))(n_{v_2}(e|G_1) + n_{v_2'}(e|G_1)) \\
\leq &\sum_{e=v_2v_2'\in E(H_2)} (d_{G_2}(v_2) + d_{G_2}(v_2'))(n_{v_2}(e|G_2) + n_{v_2'}(e|G_2)) \\
< &\sum_{e=v_2v_2'\in E(H_2)} (d_{G_3}(v_2) + d_{G_3}(v_2'))(n_{v_2}(e|G_3) + n_{v_2'}(e|G_3)).
\end{aligned}$$

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

$$\begin{aligned}&\sum_{e=xy\in E(P_n)} (d_{G_1}(x) + d_{G_1}(y))(n_x(e|G_1) + n_y(e|G_1))\\ &< \sum_{e=xy\in E(T_n)} (d_{G_2}(x) + d_{G_2}(y))(n_x(e|G_2) + n_y(e|G_2))\\ &< \sum_{e=xy\in E(S_n)} (d_{G_3}(x) + d_{G_3}(y))(n_x(e|G_3) + n_y(e|G_3)).\end{aligned}$$

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

Similarly, we can prove $PI_w(G_2) < PI_w(G_3)$. The proof completes. □

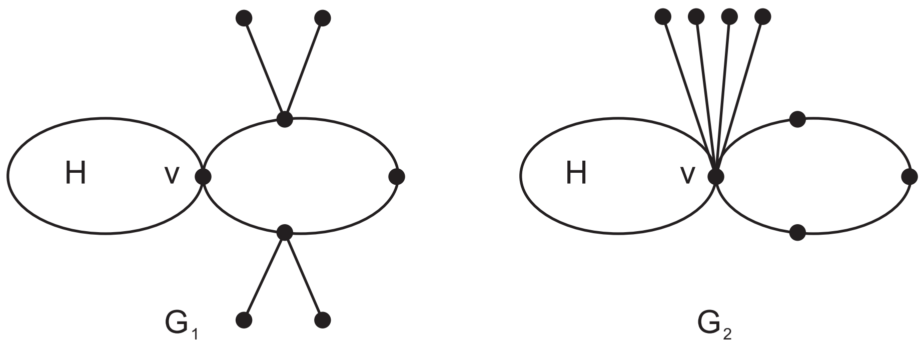

Figure 4: $PI_w(G_1) < PI_w(G_2)$.

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_1 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_1 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*

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

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 $1 \le i \le r-1$ and $\sum_{i=1}^{r-1} t_i = t$.

Note that $d_{G_1}(v) = d_{G_2}(v) - t$. 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 $n_v(e|G_1) + n_{v'}(e|G_1) = n_v(e|G_2) + n_{v'}(e|G_2)$. So

$$\begin{aligned}&\sum_{e=vv'\in E(H)} (d_{G_1}(v) + d_{G_1}(v'))(n_v(e|G_1) + n_{v'}(e|G_1)) - \sum_{e=vv'\in E(H)} (d_{G_2}(v) + d_{G_2}(v'))(n_v(e|G_2) + n_{v'}(e|G_2))\\ &\quad < 0.\end{aligned}$$

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

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

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 $n_v(e|G_2) + n_{v'}(e|G_2) = n$.

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

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

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

For the edge $e = v_i v_{i+1}$ $(0 \le i \le r-1)$ of C_r in G_2, $d_{G_2}(v_i) + d_{G_2}(v_{i+1}) = 4$ when $1 \le i \le r-2$, $d_{G_2}(v_0) + d_{G_2}(v_1) = d_{G_2}(v) + 2$ 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, $n_{v_i}(e|G_2) + n_{v_{i+1}}(e|G_2) = n$.

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

Now we are ready to compare $PI_w(G_1)$ with $PI_w(G_2)$.

$$\begin{aligned}PI_w(G_1) - PI_w(G_2) = &\sum_{e=vv'\in E(H)} (d_{G_1}(v) + d_{G_1}(v'))(n_v(e|G_1) + n_{v'}(e|G_1))\\ &+ \sum_{i=1}^{r-1}\sum_{e=v_i v_i'\in E(G_1)} (d_{G_1}(v_i) + d_{G_1}(v_i'))(n_{v_i}(e|G_1) + n_{v_i'}(e|G_1))\\ &+ \sum_{i=0}^{r-1}(d_{G_1}(v_i) + d_{G_1}(v_{i+1}))(n_{v_i}(e|G_1) + n_{v_{i+1}}(e|G_1))\\ &- \sum_{e=vv'\in E(H)} (d_{G_2}(v) + d_{G_2}(v'))(n_v(e|G_2) + n_{v'}(e|G_2))\\ &- \sum_{e=vv'\in E(G_2)\setminus E(H), d_{G_2}(v')=1} (d_{G_2}(v) + d_{G_2}(v'))(n_v(e|G_2) + n_{v'}(e|G_2))\\ &- \sum_{i=0}^{r-1}(d_{G_2}(v_i) + d_{G_2}(v_{i+1}))(n_{v_i}(e|G_2) + n_{v_{i+1}}(e|G_2))\\ &< 0.\end{aligned}$$

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

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

The proof completes. □

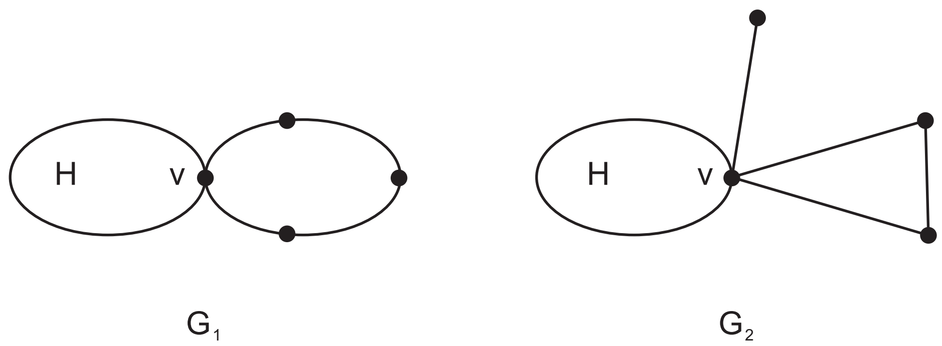

Figure 5: $PI_w(G_1) < PI_w(G_2)$.

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*

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

Proof. Suppose $|G_1| = |G_2| = n$ without of generality. Note that $d_{G_1}(v) = d_{G_2}(v) - (r-3)$. 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 $n_v(e|G_1) + n_{v'}(e|G_1) = n_v(e|G_2) + n_{v'}(e|G_2)$. So

$$\sum_{e=vv' \in E(H)} (d_{G_1}(v) + d_{G_1}(v'))(n_v(e|G_1) + n_{v'}(e|G_1)) - \sum_{e=vv' \in E(H)} (d_{G_2}(v) + d_{G_2}(v'))(n_v(e|G_2) + n_{v'}(e|G_2)) < 0.$$

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

$$\sum_{i=0}^{r-1} (d_{G_1}(v_i) + d_{G_1}(v_{i+1}))(n_{v_i}(e|G_1) + n_{v_{i+1}}(e|G_1)) = 4(r-1) + (n-1)[2(d_{G_1}(v) + 2) + 4(r-3)].$$

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

$$\sum_{i=0}^{r-1} (d_{G_1}(v_i) + d_{G_1}(v_{i+1}))(n_{v_i}(e|G_1) + n_{v_{i+1}}(e|G_1)) = n[2(d_{G_1}(v) + 2) + 4(r-2)].$$

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

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

For the edges in C_3 of G_2,

$$\sum_{i=0}^{2} (d_{G_2}(v_i) + d_{G_2}(v_{i+1}))(n_{v_i}(e|G_2) + n_{v_{i+1}}(e|G_2)) = 4 \times 2 + 2(d_{G_2}(v) + 2)(n-1) = 8 + 2(d_{G_1}(v) + r - 1)(n-1).$$

It is now straightforward to show that $PI_w(G_2) - PI_w(G_1) > 0$. The proof completes. □

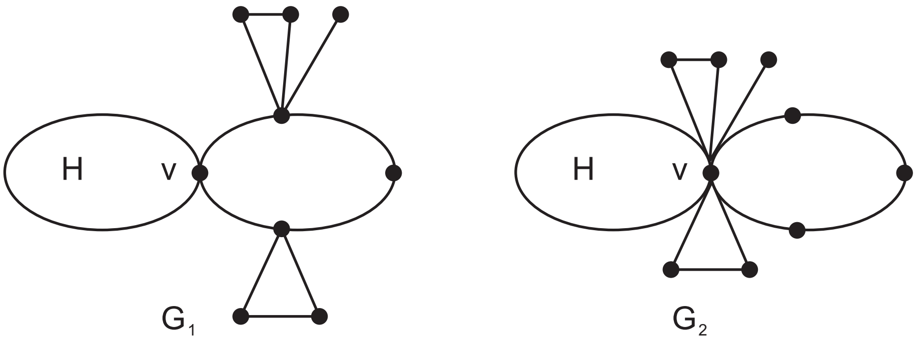

Figure 6: $PI_w(G_1) < PI_w(G_2)$.

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 $G \in \mathcal{CA}(n, s)$, $PI_w(G) \leq PI_w(S_n^{+,s})$ and the equality holds if and only if $G \cong S_n^{+,s}$.

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

3. The lower bound

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

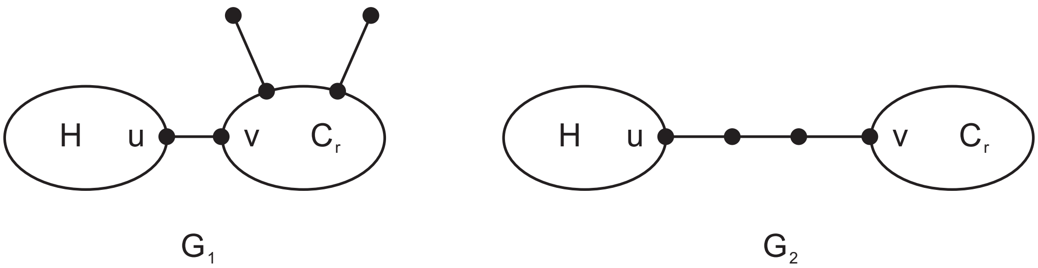

Figure 7: $PI_w(G_1) > PI_w(G_2)$.

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 $G_2 = H(u)P_{s+t+1}(v)C_r$. Note that $|G_1| = |G_2|$. See Figure 7. Then we have*

$$PI_w(G_1) > PI_w(G_2).$$

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

$$\begin{aligned} PI_w(G_1) - PI_w(G_2) &= 4tn + \sum_{i=0}^{r-1}(d_{G_1}(v_i) + d_{G_1}(v_{i+1}))(n_{v_i}(e|G_1) + n_{v_{i+1}}(e|G_1)) \\ &- 4tn - \sum_{i=0}^{r-1}(d_{G_2}(v_i) + d_{G_2}(v_{i+1}))(n_{v_i}(e|G_2) + n_{v_{i+1}}(e|G_2)) \\ &= 6[\sum_{i=1}^{r-1}(t_i + 1) + \sum_{i=1}^{r-1}(n - t_i - 1)] - [4(r-1) + (n-1)(5 \times 2 + 4(r-3))] \\ &> 0. \end{aligned}$$

When r is even, $PI_w(G_1) > PI_w(G_2)$ can be proved similarly. This completes the proof. □

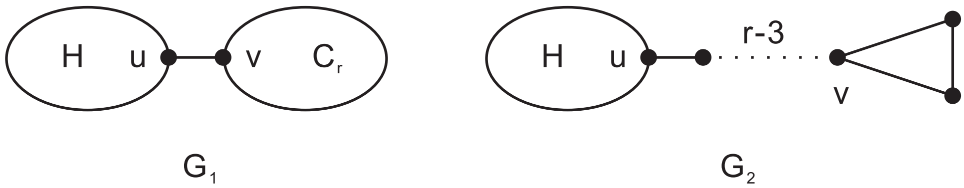

Figure 8: $PI_w(G_1) \geq PI_w(G_2)$. The equality holds if and only if r is odd.

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*

$$PI_w(G_1) \geq PI_w(G_2),$$

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 $v_0(v), v_1, v_2, \cdots, v_{r-1}$ 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.

$$\begin{aligned} PI_w(G_1) - PI_w(G_2) &= \sum_{i=0}^{r-1}(d_{G_1}(v_i) + d_{G_1}(v_{i+1}))(n_{v_i}(e|G_1) + n_{v_{i+1}}(e|G_1)) \\ &- 4(r-3)n - \sum_{i=0}^{2}(d_{G_2}(v_i) + d_{G_2}(v_{i+1}))(n_{v_i}(e|G_2) + n_{v_{i+1}}(e|G_2)). \end{aligned}$$

When r is even,

$$PI_w(G_1) - PI_w(G_2) = [2 \times 5 + 4(r-2)]n - 4(r-3)n - 2 \times 5(n-1) - 4 \times 2$$
$$> 0.$$

When r is odd,

$$PI_w(G_1) - PI_w(G_2) = [2 \times 5 + 4(r-3)](n-1) + 4(r-1) - 4(r-3)n - 2 \times 5(n-1) - 4 \times 2$$
$$= 0.$$

When $s = 0$, H and C_r share a common vertex u. $PI_w(G_1) > PI_w(G_2)$ can be proved similarly in this case. The proof completes. □

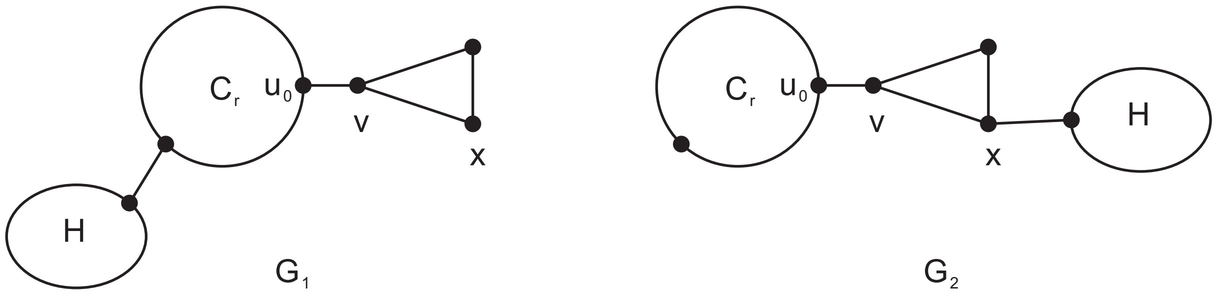

Figure 9: $PI_w(G_1) > PI_w(G_2)$.

Lemma 3.3. *Let C_r be a cycle with $r \geq 4$ and $u_0, u_1, \cdots, u_{r-1}$ are the vertices of C_r subsequently. Let H_0 be a cactus graph such that $\delta(H_0) \geq 2$ and all cycles 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 ≥ 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 $u_i w$ for any $w \in V(H)$ and adding the edge xw. See Figure 9. Then we have*

$$PI_w(G_1) > PI_w(G_2).$$

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 ≥ 1 for simplicity. Note that $d_{G_1}(u_i) = d_{G_2}(x)$.

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 $u_i u_{i-1}, u_i u_{i+1}, vx, vy, xy$ respectively.

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

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

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

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

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

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 ($1 \le j \le r-1$ and $j \ne i$) where u_j is a cut vertex, the conclusion is still correct.

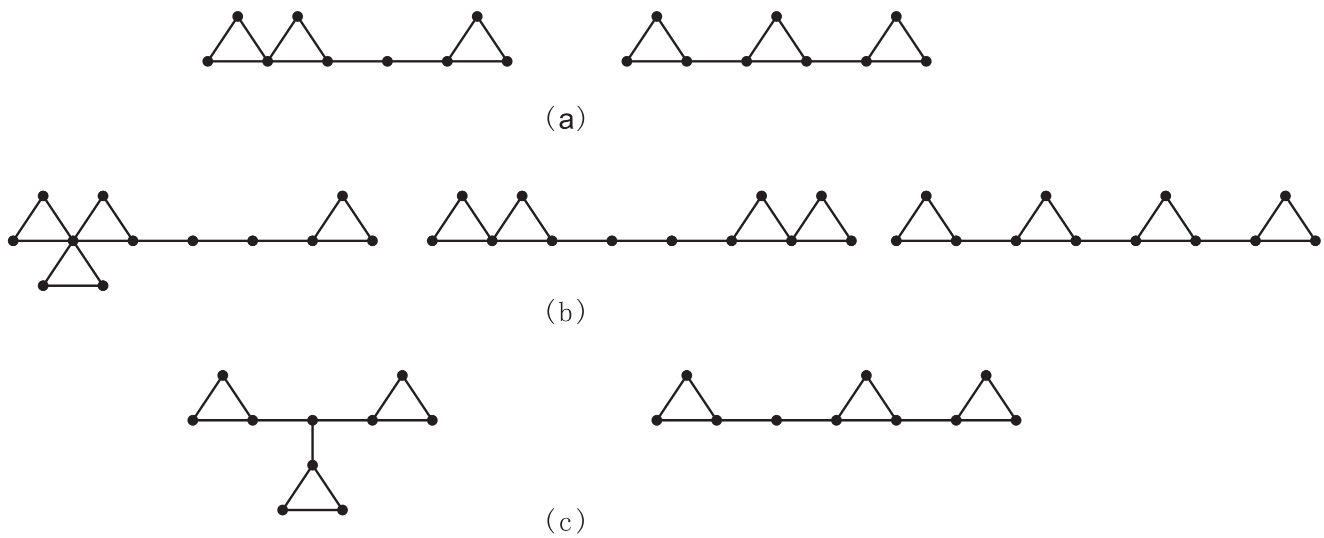

Figure 10: $PI_w(G_1) \ge PI_w(G_2)$. The equality holds if and only if $r = 3$.

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

Proof. [Proof of Theorem 1.2] Let $G \in \mathcal{CA}(n,s)$. From Lemma 2.1, Lemma 3.1, Lemma 3.2 and Lemma 3.3, we can assume that $\delta(G) \ge 2$ and all cycles of G are triangles. If $G \in \mathcal{T}(n,s)$, nothing needs to be proved. If $G \notin \mathcal{T}(n,s)$, 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. □

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