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Research article

On the maximum Graovac-Pisanski index of bicyclic graphs

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Abstract: For a simple graph $G = (V(G), E(G))$, the Graovac-Pisanski index of G is defined as

$$GP(G) = \frac{|V(G)|}{2|\operatorname{Aut}(G)|} \sum_{u \in V(G)} \sum_{\alpha \in \operatorname{Aut}(G)} d_G(u, \alpha(u)),$$

where $\operatorname{Aut}(G)$ is the automorphism group of G and $d_G(u, v)$ is the length of a shortest path between the two vertices u and v in G. Obviously, $GP(G) = 0$ if G has no nontrivial automorphisms. Let $B_n^{3,3}$ be the graph consisting of two disjoint 3-cycles with a path of length $n - 5$ joining them. In this article, we prove that among all those n-vertex bicyclic graphs in which every edge lies on at most one cycle, $B_n^{3,3}$ has the maximum Graovac-Pisanski index.

Keywords: modified Wiener index; Graovac-Pisanski index; automorphism; orbit; bicyclic graphs
Mathematics Subject Classification: 05C12, 05C25

1. Introduction

Molecular topological indices are graph invariants and have various applications in mathematical chemistry. In recent decades, a number of topological indices have been extensively studied such as the Randić index [2,16] and Estrada index [19,20]. One of the most well-known molecular topological indices is the Wiener index [23], which was developed by Harry Wiener in 1947. It is described as the sum of the distance between each pair of vertices in a graph. Since Wiener's foundational work, several iterations of the Wiener index have been developed. One of these is the Graovac-Pisanski index [7], which is similarly based on distances. Since the symmetry of a graph affects the characteristics of a molecule [15], this index has an advantage over other distance-based indices.

Let $G = (V(G), E(G))$ be a graph. The *distance* $d_G(u, v)$ between two vertices u and v in G is the length of the shortest path between u and v. An *automorphism* of G is a permutation α of its vertex set which preserves adjacency: If $uv \in E(G)$, then $\alpha(u)\alpha(v) \in E(G)$. For every graph G, the set $Aut(G)$

containing all of its automorphisms is known as the *automorphism group* of G. The Graovac-Pisanski index of G is defined as

$$GP(G) = \frac{|V(G)|}{2|Aut(G)|} \sum_{u \in V(G)} \sum_{\alpha \in Aut(G)} d_G(u, \alpha(u)).$$

It was shown in [1] that the quotient of the Wiener index and the Graovac-Pisanski index is strongly correlated with the topological efficiency for some nanostructures. The topological efficiency was introduced in [3] as a tool for the classification of the stability of molecules. A correlation between the Graovac-Pisanski index and the melting points of some families of hydrocarbon molecules was established in [5]. For more recent studies on the Graovac-Pisanski index of some linear polymers, nanostructures and some particular fullerenes, see [9, 13, 14, 18, 21].

The mathematical properties of the Graovac-Pisanski index were also investigated. Some general results on the Graovac-Pisanski index were obtained [8, 12, 17]. The exact value of the Graovac-Pisanski index for Sierpiński graphs were obtained [6] and the closed formulae for carbon nanotubes were calculated [22]. Note that if there is no nontrivial automorphisms in a graph G, then $GP(G) = 0$. Hence, it only makes sense to consider the maximum value of $GP(G)$. Denoted by P_n/C_n the path/cycle of length n. Let H_n be the graph produced from $P_n - 5$ by adding two pendant vertices to either end of $P_n - 5$. Knor et al. considered the maximum Graovac-Pisanski indices of trees and unicyclic graphs [10, 11], and they proposed the following conjecture.

Conjecture 1.1. *[10,11] Among all graphs on n vertices, P_{n-1}, H_n and C_n have the maximum Graovac-Pisanski index if $n \geq 8$.*

For a connected graph G, we define the 2-*core* of G, denoted by $B(G)$, as the graph obtained from G by recursively deleting pendant vertices until no pendant vertices remain. We denote by $B_n^{p,q}$ $(p, q \geq 3)$ the graph obtained from the two cycles C_p and C_q by adding a $P_{n+1-p-q}$ between them. If G contains some $B_n^{p,q}$ as a 2-core, then we say G is an ∞-shape bicycle graph.

In this article, we concentrate on the maximum Graovac-Pisanski index over all connected ∞-shape bicycle graphs and prove the following theorem, which implies Conjecture 1.1 is true for ∞-shape bicyclic graphs.

Theorem 1.2. *Among all connected ∞-shape bicyclic graphs on n vertices, only $B_n^{3,3}$ has the maximum Graovac-Pisanski index and*

$$GP(B_n^{3,3}) = \begin{cases} \frac{n^3}{8} - \frac{5n}{8}, & if\ n\ is\ odd; \\ \frac{n^3}{8} - \frac{n}{2}, & if\ n\ is\ even. \end{cases}$$

2. Preliminaries

We focus only on simple connected graphs that are finite, undirected and unlabelled in this article. Let $G = (V(G), E(G))$ be a graph. For $S \subseteq V(G) \cup E(G)$, we denote by $G[S]$ the subgraph induced by S, and $G - S$ the subgraph obtained from G by deleting S. For a vertex u in G, the *orbit* which contains u is the vertex set $V_u = \{\alpha(u) | \alpha \in Aut(G)\}$ and u is called the *representative* of V_u. The *order* of an orbit is the number of vertices it contains. We denote by $W_{V_u}(u) = \sum_{v \in V_u} d_G(u, v)$. Note that, for each vertex $x \in V_u$, the value of $W_{V_u}(x)$ is same.

Let $V_1, \cdots, V_t$ be all the orbits determined by $Aut(G)$ in G with the representatives $v_1, \cdots, v_t$, respectively. There is a simple expression of the Graovac-Pisanski index in terms of orbits,

$$GP(G) = \frac{|V(G)|}{2} \sum_{i=1}^{t} W_{V_i}(v_i) = \frac{|V(G)|}{2} GP_a(G), \tag{1}$$

where $GP_a(G) = \sum_{i=1}^{t} W_{V_i}(v_i)$ (see [4]).

Example 2.1. Let G_i be the graph as depicted in Figure 1, where $1 \leq i \leq 5$ (each orbit in G_i is colored with a different color). By Eq (1), we can obtain that

$$GP(G_1) = \frac{5}{2} \times (4+2) = 15, \;\; GP(G_2) = \frac{5}{2} \times (1+1+0) = 5,$$

$$GP(G_3) = \frac{5}{2} \times (2+0+0+0) = 5, \;\; GP(G_4) = \frac{5}{2} \times (1+0+0+0) = \frac{5}{2},$$

$$GP(G_5) = \frac{5}{2} \times (5+0) = \frac{25}{2}.$$

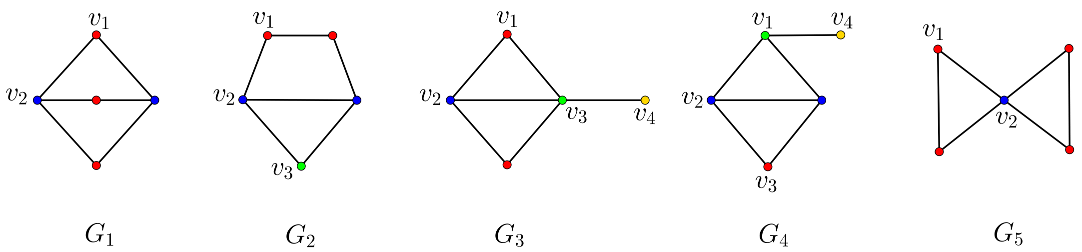

Figure 1. The graphs G_1-G_5 and their orbits.

Obviously, if we consider the maximum value of the Graovac-Pisanski index of an n-vertex graph G, we only need to consider the maximum value of $GP_a(G)$ by (1).

Theorem 2.2. *[10] Let T be a tree on n vertices, then*

$$GP_a(T) \leq \begin{cases} \frac{n^2-1}{4}, & \text{when } n \text{ is odd;} \\ \frac{n^2}{4}, & \text{when } n \text{ is even.} \end{cases}$$

Moreover, when $n \geq 8$, then the equality holds if and only if $G \cong P_{n-1}$ or $G \cong H_n$.

A bicycle graph G is the graph with the property $|E(G)| = |V(G)| + 1$. It is well know that there are two types of bicyclic graphs. We call G a Θ-shape bicycle graph if the two cycles in G share one common edge, otherwise, we call G an ∞-shape bicyclic graph. For $V_1, V_2 \subseteq V(G)$, if $|V_1| = |V_2|$ and there exists a permutation $\alpha \in Aut(G)$ such that $\alpha(x) \in V_2$ for any $x \in V_1$, then we denote $\alpha(V_1) = V_2$.

Observation 2.3. *Let G be an ∞-shape bicycle graph, and let $B := B(G)$ be the 2-core of G which is formed from two cycles C_p and C_q with a (u, v)-path P_l joining them, where $u \in V(C_p)$ and $v \in V(C_q)$. Suppose there is some $\alpha \in Aut(G)$ such that $\alpha(V(C_p)) = V(C_q)$. Then for any vertex $r \in V(B)$, r is in an orbit V_r of order 1 or 2 or 4. Moreover, $|V_r| = 1$ only if l is even and r is the vertex in the (u, v)-path P_l with $d_G(r, u) = \frac{l}{2}$.*

Proof. Since u and v are the only two vertices with degree 3 in the 2-core B of G, we have $\gamma(u) = v$ or $\gamma(u) = u$ for any $\gamma \in Aut(G)$. Recall that γ is a permutation which preserves adjacency, hence for every $x \in V(B)$,

$$d_G(x, u) = d_G(\gamma(x), \gamma(u)).$$

Let $V_r \subseteq V(B)$ be an orbit with representative r.

Case 1. $r \in V(C_p) \cup V(C_q)$.

Without loss of generality, we assume $r \in V(C_p)$. Since $\alpha(V(C_p)) = V(C_q)$, then $\alpha(u) = v$. Hence, the vertex $\alpha(r) \in V(C_q)$ with $d_G(\alpha(r), v) = d_G(r, u)$ is in V_r. Let $w \in V(C_p)$ be the vertex different from r with $d_G(r, u) = d_G(w, u)$ (if it exists). If there exists $\beta \in Aut(G)$ such that $\beta(r) = w$, then

$$V_r = \{r, w, \alpha(r), \alpha(w)\}$$

is an orbit of order 4. If for any $\gamma \in Aut(G)$, $\gamma(r) \neq w$ or w does not exist, then $V_r = \{r, \alpha(r)\}$ is an orbit of order 2.

Case 2. $r \in V(P_l)$.

Obviously, $\gamma(r) \in V(P_l)$ for any $\gamma \in Aut(G)$. If l is even and $r \in V(P_l)$ is the vertex with $d_G(r, u) = \frac{l}{2}$, then r is unique vertex in B with $d_G(r, u) = d_G(r, v)$. Hence, for any $\gamma \in Aut(G)$, $\gamma(r) = r$ and $V_r = \{r\}$ is the unique orbit of order 1. Otherwise, $V_r = \{r, \alpha(r)\}$ is an orbit of order 2, where $\alpha(r) \in V(P_l)$ with $d_G(r, u) = d_G(\alpha(r), v)$. □

3. The maximum $GP_a(G)$ of ∞-shape bicycle graphs

In this section, unless otherwise specified, we always let G be an ∞-shape bicyclic graph of order n, and $B := B(G)$ be the 2-core of G which is formed from two cycles C_p, C_q with a (u, v)-path P_l joining them, where $u \in V(C_p)$ and $v \in V(C_q)$.

Let T_w be a component of $G - E(B)$, where $w \in V(B)$. A tree T_w in G is *trivial* if $|V(T_w)| = 1$. Obviously, $G = B$ when all trees T_w are trivial. We remark that all the rooted trees T_w with root w in the same orbit $V_w \subseteq V(B)$ are mutually isomorphic. A subgraph of G isomorphic to a path is a *ray*, if its first vertex has degree at least 3 in G, its last vertex has degree 1 in G, and all the other vertices have degree 2 in G.

Lemma 3.1. *Let G be a connected tree or ∞-shape bicyclic graph and let k be an integer larger than 1. Suppose V_r is an orbit of G with representative r and there is a partition $V_1, V_2, \cdots, V_k$ of V_r such that for any vertex $x \in V_i$ $(1 \leq i \leq k)$, the value of $W_{V_i}(x)$ is same. Then $W_{V_r}(r) \geq \sum_{i=1}^{k} W_{V_i}(x)$.*

Proof. Since the value of $W_{V_i}(x)$ is the same for each vertex $x \in V_i$, we choose the vertex r_i which is closest to r in each V_i as the representative for $1 \leq i \leq k$. Obviously, if we prove that $d_G(r, x) \geq d_G(r_i, x)$ for every vertex $x \in V_i$, then we have $W_{V_r}(r) \geq \sum_{i=1}^{k} W_{V_i}(r_i) = \sum_{i=1}^{k} W_{V_i}(x)$. Note that $W_{V_i}(r_i) = 0$ if

$V_i = \{r_i\}$, hence we may assume each V_i contains at least two vertices for $1 \leq i \leq k$. Let x be an arbitrary vertex in $V_i \setminus \{r_i\}$, where $1 \leq i \leq k$.

Case 1. G is a tree.

Let T be the tree with the minimum number of vertices among all subtrees of G that contain r, r_i, x as leafs. It is known that every tree has either 1 or 2 central vertices. Since r, r_i, x are in the same orbit V_r, they are equidistant from some central vertex of T.

Denote by z the central vertex in T that is closest to r. Recall that r_i is the vertex closest to r in V_i. Hence, if there is a subtree $T' \subseteq T$ with leafs r, r_i and central vertex z' such that $d_G(z', r) \leq d_G(z, u)$, then

$$d_G(r, x) = d_G(r, z') + d_G(z', x) = d_G(r_i, z') + d_G(z', x) = d_G(r_i, x).$$

Otherwise, there is a subtree $T'' \subseteq T$ with leafs r_i, x and central vertex z'' such that $d_G(z'', r) > d_G(z, r)$. Note that $d_G(z'', x) \leq d_G(z, r)$. Hence,

$$d_G(r, x) = d_G(z'', r) + d_G(z'', x) > d_G(z, r) + d_G(z'', x) \geq 2d_G(z'', x) = d_G(r_i, x).$$

Therefore, we always have $d_G(r, x) \geq d_G(r_i, x)$ for any vertex $x \in V_i$, where $1 \leq i \leq k$.

Case 2. G is an ∞-shape bicyclic graph.

We may assume that r is in the root tree T_w, where $w \in V(B)$. Note that w is in an orbit $V_w \subseteq V(B)$ with order 1, 2 or 4, and by Observation 2.3, $|V_w| = 4$ only if there exists some $\alpha \in Aut(G)$ such that $\alpha(V(C_p)) = V(C_q)$. Obviously, if $|V_w| = 1$, then r, r_i and x are in the same rooted tree T_w. Hence, by case 1, $d_G(r, x) \geq d_G(r_i, x)$ for any vertex $x \in V_i$. Thus, we may assume $|V_w| = 2$ or 4 in the following.

We first consider $r_i \in V(T_w)$. If $x \in V(T_w)$, then by case 1, $d_G(r, x) \geq d_G(r_i, x)$. If $x \in V(T_{w_1})$, where $w_1 \in V_w \setminus \{w\}$, then

$$d_G(r, x) = d_G(r, w) + d_G(w, w_1) + d_G(w_1, x).$$

Since r, r_i, x are in the same orbit V_r,

$$d_G(r, w) = d_G(r_i, w) = d_G(x, w_1).$$

Hence,

$$d_G(r, x) = d_G(r_i, w) + d_G(w, w_1) + d_G(w_1, x) = d_G(r_i, x).$$

Therefore, we have $d_G(r, x) \geq d_G(r_i, x)$.

Now, we consider $r_i \notin V(T_w)$. Obviously, if x and r_i are in the same root tree, then $d_G(r, x) > d_G(r_i, x)$. Hence, we assume x and r_i are in different root trees. And since r_i is the vertex in V_i closest to r, $x \notin V(T_w)$. It follows that $|V_w| = 4$, say $V_w = \{w, w_1, w_2, w_3\}$. Without loss of generality, we may assume $\{w, w_1\} \subseteq V(C_p)$ and $\{w_2, w_3\} \subseteq V(C_q)$. If $r_i \in V(T_{w_1})$, then $x \in V(T_{w_j})$ with

$$d_G(r, w) = d_G(r_i, w_1) = d_G(x, w_j),$$

where $2 \leq j \leq 3$. Note that

$$d_G(w, w_j) = d_G(w_1, w_j),$$

where $2 \leq j \leq 3$. Hence,

$$d_G(r, x) = d_G(r, w) + d_G(w, w_j) + d_G(w_j, x) = d_G(r_i, w_1) + d_G(w_1, w_j) + d_G(w_j, x) = d_G(r_i, x).$$

If $r_i \in V(T_{w_j})$, say $r_i \in V(T_{w_2})$, then $x \in V(T_{w_3})$ as r_i is the vertex in V_i closest to r. Note that $d_G(w, w_3) \geq d_G(w_2, w_3)$. Hence,

$$d_G(r, x) = d_G(r, w) + d_G(w, w_3) + d_G(w_3, x) \geq d_G(r_i, w_2) + d_G(w_2, w_3) + d_G(w_3, x) = d_G(r_i, x).$$

Therefore, we always have $d_G(r, x) \geq d_G(r_i, x)$ for any vertex $x \in V_i$. □

We now introduce some graph operations. By the graph operations of *cutting down* a rooted tree T_x in G and *attaching* a path P_l to $y \in V(G)$, we mean deleting the vertices $V(T_x) \setminus \{x\}$ in G and identifying one end of P_l to y, respectively. By the graph operation of *changing* a rooted tree T_x to a path, we mean cutting down T_x and then attaching a path of order $|V(T_x)|$ to x.

Lemma 3.2. *Let $s \geq 1$ be an integer and let G be an ∞-shape bicycle graph with the 2-core $B := B(G)$. Suppose $V_{v_1} = \{v_1, v_2, \cdots, v_{s+1}\} \subseteq V(B)$ is an orbit and each vertex $v_i \in V_{v_1}$ is the root of a nontrivial tree T_{v_i}, where $1 \leq i \leq s+1$. Let G' be the graph obtained from G by changing each T_{v_i} to a path for $1 \leq i \leq s+1$. Then, $GP_a(G) \leq GP_a(G')$.*

Proof. We will prove $GP_a(G) \leq GP_a(G')$ through a series of graph operations. Note that since the roots of each T_{v_i} ($1 \leq i \leq s+1$) are in the same orbit V_{v_1}, all T_{v_i} in G are isomorphic. If each T_{v_i} is a ray, then $G = G'$. Hence, each T_{v_i} contains at least two vertices with degree more than 2. Let $u_{i1}, \ldots, u_{ir}$ be the vertices in $V(T_{v_i})$ that are furthest away from v_i with degree at least 3 and lie in the same orbit of G, where $1 \leq i \leq s+1$ and $r \geq 1$. Then $V_{u_{11}} = \{u_{11}, u_{12}, \cdots, u_{1r}, \cdots, u_{(s+1)r}\}$ is an orbit of G.

Let $S_{u_{ij}} \subseteq G$ be the graph induced by the vertices contained in all the rays with u_{ij} as the first vertex for $1 \leq i \leq s+1$ and $1 \leq j \leq r$. Obviously, all $S_{u_{ij}}$ are isomorphic and for any two distinct vertices $x \in S_{u_{ij}}$ and $y \in S_{u_{i'j'}}$, if the rays containing x and y are of equal length and $d_G(x, u_{ij}) = d_G(y, u_{i'j'})$, then x and y are in the same orbit, where $1 \leq i \leq i' \leq s+1$ and $1 \leq j \leq j' \leq r$. Now, we consider the following two cases.

Case 1. Each $S_{u_{ij}}$ has at least two rays of the same length, where $1 \leq i \leq s+1$ and $1 \leq j \leq r$.

Recall that all $S_{u_{ij}}$ are isomorphic, hence we may assume there are $k (k \geq 2)$ rays in each $S_{u_{ij}}$ with the same length l for $1 \leq i \leq s+1$ and $1 \leq j \leq r$. Let G_1 be the graph obtained from G by cutting down all the k rays of length l in each $S_{u_{ij}}$ and attaching a path P_{kl} to each u_{ij} (see Figure 2(a)). Denote by $S'_{u_{ij}} \subseteq G_1$ the graph obtained from $S_{u_{ij}}$ after the graph operation, where $1 \leq i \leq s+1$ and $1 \leq j \leq r$.

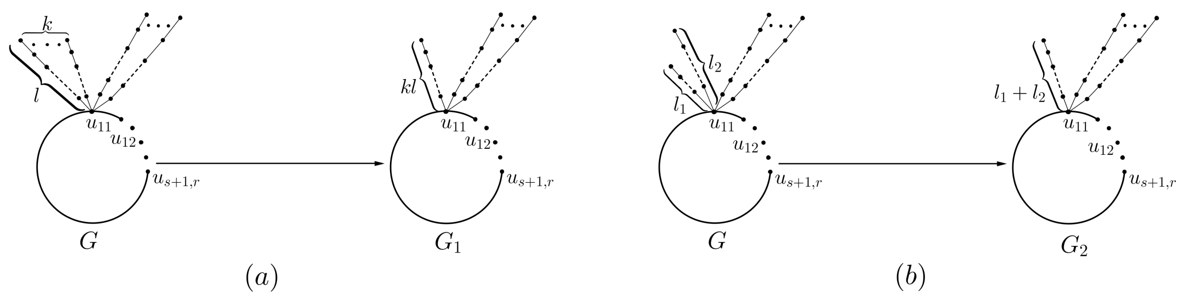

Figure 2. The process of constructing graphs G_1 and G_2.

Note that for each orbit V_u which contains the vertices in the rays of length kl in each $S'_{u_{ij}} \subseteq G_1$, V_u may also contains the vertices in the rays of length kl in G if such rays exist in some rooted tree isomorphic to T_{v_i} in G. We denote by V'_u the subset of each V_u which only contains the vertices in the path P_{kl} of each $S'_{u_{ij}} \subseteq G_1$, where $1 \le i \le s+1$ and $1 \le j \le r$.

Let $\mathcal{V}$ be the set consisting of the orbits which contain the vertices in the $kr(s+1)$ rays of length l in each $S_{u_{ij}} \subseteq G$. Let $\mathcal{V}'$ be the set consisting of the sets V'_u which contain the vertices in the $r(s+1)$ rays of length kl in each $S'_{u_{ij}} \subseteq G_1$. For convenience, for any set in $\mathcal{V}$ or $\mathcal{V}'$, we always choose the vertex in $S_{u_{11}}$ or $S'_{u_{11}}$ as representative, respectively. According to the distance between the representatives of each set to u_{11}, we can obtain $|\mathcal{V}| = k$ and $|\mathcal{V}'| = kl$.

Note that, after the process of constructing G_1 from G, some orbits of G may merge into a new orbit of G_1 and the orbit V_u of G_1 may also contains some orbits of G. By Lemma 3.1, we can see that the vertices in these orbits will increase the value of $GP_a(G)$ after the process. Hence, if we can prove $\sum_{V_x \in \mathcal{V}} W_{V_x}(x) \le \sum_{V'_y \in \mathcal{V}'} W_{V'_y}(y)$, where V_x is the orbit in $\mathcal{V}$ with representative x and V'_y is the set in $\mathcal{V}'$ with representative y, then we have $GP_a(G_1) \ge GP_a(G)$.

Let V_f be the orbit in $\mathcal{V}$ which contains the representative x_f in some ray of length l in $S_{u_{11}}$ with $d_G(x_f, u_{11}) = f$ $(1 \le f \le l)$, and let V'_t be the set in $\mathcal{V}'$ which contains the representative y_t in the path P_{kl} of $S'_{u_{11}}$ with $d_{G_1}(y_t, u_{11}) = t$ $(1 \le t \le kl)$. Then,

$$\begin{aligned}\sum_{t=1}^{kl} W_{V'_t}(y_t) - \sum_{f=1}^{l} W_{V_f}(x_f) &= \sum_{t=1}^{kl} \Big(2t(r-1) + 2trs + W_{V_{u_{11}}}(u_{11})\Big) - \sum_{f=1}^{l} \Big(2fkr(s+1) - 2f + kW_{V_{u_{11}}}(u_{11})\Big) \\ &= k^2(l^2rs + l^2r - l^2) - k(l^2rs + l^2r + l) + l^2 + l \\ &\ge l^2(2rs + 2r - 3) - l \ge 0,\end{aligned}$$

as $k \ge 2, s \ge 1, l \ge 1$ and $r \ge 1$. Therefore, $GP_a(G_1) \ge GP_a(G)$.

Case 2. All the rays in each $S_{u_{ij}}$ have different length, where $1 \le i \le s+1$ and $1 \le j \le r$.

We may assume that in each $S_{u_{ij}}$, there are two rays of length l_1 and l_2 respectively, where $l_2 > l_1$. Let G_2 be the graph obtained from G by cutting down the ray of length l_1 in each $S_{u_{ij}}$ and attaching a path of length l_1 to the end vertex of the ray of length l_2 in each $S_{u_{ij}}$, where $1 \le i \le s+1$ and $1 \le j \le r$ (see Figure 2(b)). Denote by $S''_{u_{ij}} \subseteq G_2$ the graph obtained from $S_{u_{ij}}$ after the graph operation. For each orbit V_u which contains the vertices in the rays of length $l_1 + l_2$ in each $S''_{u_{ij}} \subseteq G_2$, we denote by V''_u the subset of each V_u that contains only the vertices in rays of length $l_1 + l_2$ that are not in G, where $1 \le i \le s+1$ and $1 \le j \le r$.

Analogously to Case 1, let $\mathcal{V}$ and $\mathcal{V}'$ be the set consisting of the orbits which contain the vertices in the $r(s+1)$ rays of length l_1 and l_2 in each $S_{u_{ij}} \subseteq G$, respectively. Let $\mathcal{V}''$ be the set consisting of the sets V''_u which contain the vertices in the $r(s+1)$ rays of length $l_1 + l_2$ in each $S''_{u_{ij}} \subseteq G_2$. Denote by V_t the orbit in $\mathcal{V}$ which contains the representative x_t in some ray of length l_1 in $S_{u_{11}}$ with

$$d_G(x_t, u_{11}) = t, \quad (1 \le t \le l_1),$$

$V_{t'}$ the orbit in $\mathcal{V}'$ which contains the representative $y_{t'}$ in some ray of length l_2 in $S_{u_{11}}$ with

$$d_G(y_{t'}, u_{11}) = t', \quad (1 \le t' \le l_2),$$

and $V_{t''}$ the set in $\mathcal{V}''$ contains the representative $z_{t''}$ in some ray of length $l_1 + l_2$ in $S''_{u_{11}}$ with

$$d_{G_2}(z_{t''}, u_{11}) = t'', \ \ (1 \leq t'' \leq l_1 + l_2).$$

As we mentioned in Case 1, if some different orbits of G merge into a new orbit in G_2, then such orbits will increase the value of $GP_a(G)$. Hence, we only need to consider the difference between $\sum_{V_t \in \mathcal{V}} W_{V_t}(x_t) + \sum_{V_{t'} \in \mathcal{V}'} W_{V_{t'}}(y_{t'})$ and $\sum_{V_{t''} \in \mathcal{V}''} W_{V_{t''}}(z_{t''})$. Since $s \geq 1$, $r \geq 1$ and $l_2 > l_1 \geq 1$, we have

$$\begin{aligned}\sum_{V_{t''} \in \mathcal{V}''} W_{V_{t''}}(z_{t''}) - \left(\sum_{V_t \in \mathcal{V}} W_{V_t}(x_t) + \sum_{V_{t'} \in \mathcal{V}'} W_{V_{t'}}(y_{t'}) \right) &= \sum_{t''=l_1+1}^{l_1+l_2} W_{V_{t''}}(y_{t''}) - \sum_{t'=1}^{l_2} W_{V_{t'}}(y_{t'}) \\ &= \sum_{t''=l_1+1}^{l_1+l_2} (2t''rs + W_{V_{u_{11}}}(u_{11})) - \sum_{t'=1}^{l_2} (2t'rs + W_{V_{u_{11}}}(u_{11})) \\ &> 0.\end{aligned}$$

Therefore, $GP_a(G_2) \geq GP_a(G)$.

By repeating the two processes of constructing G_1 and G_2 from G, we can get the final result. □

For the (u, v)-path P_l in B, if l is odd, then we say the *middle* edge of P_l is the edge xy in P_l with $d_G(u, x) = d_G(y, v)$; if l is even, then we say the middle edge of P_l are the two edges incident to w, where w is the vertex in P_l with $d_G(u, w) = d_G(w, v)$. The graph operation of *subdividing* P_l k *times* means changing the middle edge of P_l to a path of length $k + 1$.

Suppose there is some $\alpha \in Aut(G)$ such that $\alpha(V(C_p)) = V(C_q)$. Let M denote the graph obtained from G by cutting down each rooted tree T_w, where $w \in V(P_l)$ and subdividing the (u, v)-path P_l by $\sum_{w \in V(P_l)}(|T_w| - 1)$ times (see Figure 3). Let F denote the graph obtained from M by changing each nontrivial rooted tree T_r to a path, where $r \in V(C_p) \cup V(C_q)$.

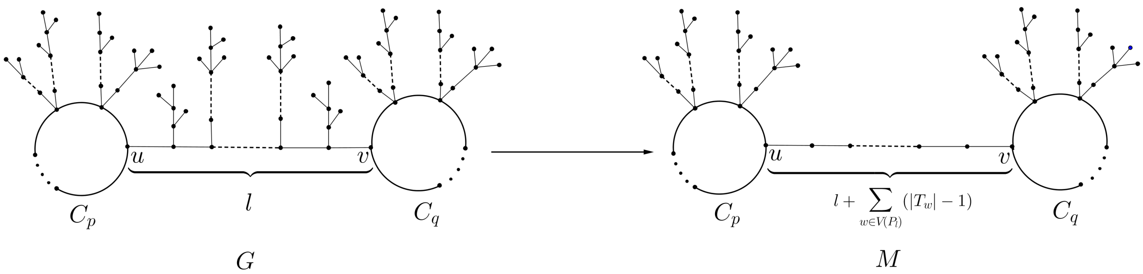

Figure 3. The process of constructing M from G.

Lemma 3.3. *If there exists some $\alpha \in Aut(G)$ such that $\alpha(V(C_p)) = V(C_q)$, then $GP_a(G) \leq GP_a(B_n^{p,p})$.*

Proof. Since $\alpha(V(C_p)) = V(C_q)$, we may assume $|V(C_p)| = |V(C_q)| = p$. Let M and F be the graphs defined above. We will show

$$GP_a(G) \leq GP_a(M) \leq GP_a(F) \leq GP_a(B_n^{p,p})$$

in the following.

We first state that $GP_a(G) \leq GP_a(M)$. Denote by $P_{l'}$ the (u, v)-path in the 2-core $B(M)$ of M. Let

$$\widetilde{V} = \{x|x \in V(T_w), w \in V(P_l) \subseteq V(G)\},\ \widehat{V} = \{x|x \in V(P_{l'}) \subseteq V(M)\}.$$

It can be seen that any orbit $V_x \subseteq V(G)$ belongs to $\widetilde{V}$ or $V(G) \setminus \widetilde{V}$ and any orbit $V_y \subseteq V(M)$ belongs to $\widehat{V}$ or $V(M) \setminus \widehat{V}$. The orbits in $V(G) \setminus \widetilde{V}$ and $V(M) \setminus \widehat{V}$ are same. Since $d_M(u, v) \geq d_G(u, v)$, by the definition of $W_{V_x}(x)$, we can directly obtain the

$$\sum_{V_x \subseteq V(G)\setminus\widetilde{V}} W_{V_x}(x) \leq \sum_{V_y \subseteq V(M)\setminus\widehat{V}} W_{V_y}(y).$$

And since $G[\widetilde{V}]$ is a tree and $G[\widehat{V}]$ is a path, by Theorem 2.2, we have

$$\sum_{V_x \subseteq \widetilde{V}} W_{V_x}(x) \leq \sum_{V_y \subseteq \widehat{V}} W_{V_y}(y).$$

Therefore,

$$\begin{aligned} GP_a(G) &= \sum_{V_x \subseteq \widetilde{V}} W_{V_x}(x) + \sum_{V_x \subseteq V(G)\setminus\widetilde{V}} W_{V_x}(x) \\ &\leq \sum_{V_y \subseteq \widehat{V}} W_{V_y}(y) + \sum_{V_y \subseteq V(M)\setminus\widehat{V}} W_{V_y}(y) = GP_a(M). \end{aligned}$$

Next, we show $GP_a(M) \leq GP_a(F)$. Recall that the orbits in $V(G) \setminus \widetilde{V}$ and $V(M) \setminus \widehat{V}$ are the same. Hence, by Observation 2.3, each orbit in $V(M) \setminus \widehat{V}$ is of order 2 or 4. Let V_r be an orbit in $V(M) \setminus \widehat{V}$ and let M' be the graph obtained from M by changing each rooted tree T_y to a path, where $y \in V_r$. Then by Lemma 3.2, we have $GP_a(M) \leq GP_a(M')$. Next, by repeating the process of constructing M' from M, we can finally get the graph F from M and we have $GP_a(M) \leq GP_a(F)$.

Finally, we show $GP_a(F) \leq GP_a(B_n^{p,p})$. We remark that any vertex

$$r \in V(C_p) \cup V(C_q) \subseteq V(B(F))$$

belongs to an orbit V_r of order 2 or 4 and each rooted tree with root in V_r is a path of same length. Let T_{t_0} be the rooted tree of minimum length among all nontrivial paths with roots in $V(C_p) \cup V(C_q)$. Denote by $V_{t_0} = \{t_0, t_1, \cdots, t_k\}$ the orbit which contains t_0, where $k \in \{1, 3\}$. Let F' be the graph obtained from F by deleting the end vertices of all paths with roots in V_{t_0} and subdividing the (u, v)-path in $B(F)$ by $|V_{t_0}|$ times (Figure 4 depicts the case with $|V_{t_0}| = 4$). Obviously, if we can show $GP_a(F) \leq GP_a(F')$, then by repeating the process of constructing F' from F, we can finally get $GP_a(F) \leq GP_a(B_n^{p,p})$.

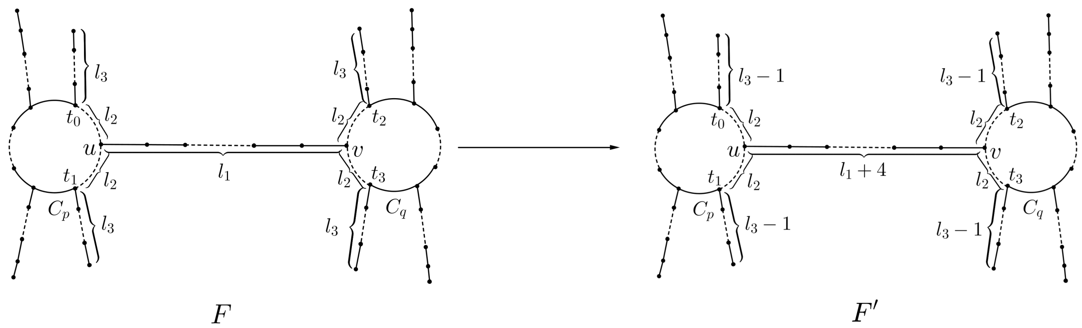

Figure 4. The process of constructing F' from F.

Let the length of the (u, v)-path in $B(F)$ be l_1. Then, $0 \le l_1 \le n-5$. Recall that $|V_{t_0}| = 4$ or 2.

Case 1. $|V_{t_0}| = 4$.

Let $V_{t_0} = \{t_0, t_1, t_2, t_3\}$ with

$$d_F(t_0, u) = d_F(t_1, u) = d_F(t_2, v) = d_F(t_3, v) = l_2.$$

Let the length of the nontrivial path rooted at t_i be l_3, where $0 \le i \le 3$. Then, $1 \le l_2 \le \lfloor \frac{p}{2} \rfloor$ and $0 \le l_3 \le \frac{n+1-2p-l_1}{4}$. Denote by V' the set consisting of the vertices closer to v in all orbits of F'. Since the length of the (u, v)-path in $B(F')$ is $l_1 + 4$, it can be seen that except the two vertices adding into the (u, v)-path, each vertex in V' contributes 4 more to $GP_a(F')$ than to $GP_a(F)$. Hence, if n is odd, then the positive contribution of the vertices in V' to $GP_a(F')$ is $\frac{n-5}{2} \times 4 + 2 + 4 = 2n - 4$; if n is even, then the positive contribution of the vertices in V' to $GP_a(F')$ is $\frac{n-4}{2} \times 4 + 1 + 3 = 2n - 4$. Note that $d_F(t_0, t_1) = \min\{p - 2l_2, 2l_2\}$. If $d_F(t_0, t_1) = p - 2l_2 \ge 1$, then

$$\begin{aligned} GP_a(F') - GP_a(F) &= 2n - 4 - [2l_3 + (p - 2l_2) + 2 \times (2l_3 + 2l_2 + l_1)] \\ &\ge 2n - 4 - 6\left(\frac{n+1-2p-l_1}{4}\right) - p - 2l_2 - 2l_1 \\ &= \frac{n - l_1}{2} + 2(p - l_2) - \frac{11}{2} > 0 \end{aligned}$$

as $n - l_1 \ge 5$ and $p - l_2 \ge 1 + l_2 \ge 2$. If $d_F(t_0, t_1) = 2l_2 \ge 2$, then

$$\begin{aligned} GP_a(F') - GP_a(F) &= 2n - 4 - [2l_3 + 2l_2 + 2 \times (2l_3 + 2l_2 + l_1)] \\ &\ge \frac{n - l_1}{2} + 3(p - 2l_2) - \frac{11}{2} > 0 \end{aligned}$$

as $p - 2l_2 \ge 2l_2 \ge 2$.

Case 2. $|V_{t_0}| = 2$.

Let $V_{t_0} = \{t_0, t_1\}$ with $d_F(t_0, u) = d_F(t_1, v) = l'_2$. Let the length of the nontrivial path rooted at t_i be l'_3, where $0 \le i \le 1$. Note that in this case, the length of the (u, v)-path in $B(F')$ is $l_1 + 2$. Hence, by a similar analysis as in Case 1, we have

$$GP_a(F') - GP_a(F) = n - 1 - (2l'_3 + 2l'_2 + l_1) \ge p - 1 > 0$$

as $2l'_3 + 2l'_2 + l_1 \le n - p$.

Therefore, by repeating the process of constructing F' from F, we can get finally get the graph $B_n^{p,q}$ from F and we have $GP_a(G) \le GP_a(B_n^{p,q})$. □

Next, we will show that Theorem 1.2 holds by proving the following theorem.

Theorem 3.4. *Let G be a connected ∞-shape bicyclic graph. Then*

$$GP_a(G) \le \begin{cases} \frac{n^2}{4} - \frac{5}{4}, & if\ n\ is\ odd; \\ \frac{n^2}{4} - 1, & if\ n\ is\ even, \end{cases}$$

and the equality holds if and only if $G \cong B_n^{3,3}$.

Proof. Recall that the 2-core B of G is formed from two cycles C_p, C_q with a (u, v)-path P_l joining them, where $u \in V(C_p)$ and $v \in V(C_q)$. Any $\gamma \in Aut(G)$ is a permutation of $V(G)$ which preserves adjacency. Hence for any vertex $r \in V(C_p)$, we have $\gamma(r) \in V(C_p)$ or $\gamma(r) \in V(C_q)$. It follows that for any $\gamma \in Aut(G)$,

$$\gamma(V(C_p)) = V(C_q)$$

or

$$\gamma(V(C_p)) = V(C_p).$$

Case 1. There exists some $\alpha \in Aut(G)$ such that $\alpha(V(C_p)) = V(C_q)$.

By Lemma 3.3, $GP_a(G) \leq GP_a(B_n^{p,p})$. Let V_1 be the set containing the vertices in the two cycles C_p in $B_n^{p,p}$ other than u and v and $V_2 = V(B_n^{p,p}) \setminus V_1$. It can be seen that any orbit in $B_n^{p,p}$ belongs to V_1 or V_2.

For each orbit $V_r \subseteq V(B_n^{p,p})$, we choose the vertex closest to u in V_r as the representative r. Denote $d = d_{B_n^{p,p}}(r, u)$. If $V_r \subseteq V_1$, then $1 \leq d \leq \lfloor \frac{p}{2} \rfloor$. By Observation 2.3, if p is even and $d = \frac{p}{2}$, then $|V_r| = 2$. Otherwise, $|V_r| = 4$. Therefore, we have

$$W_{V_r}(r) = \begin{cases} 2d + 2(2d + (n + 1 - 2p)) = 2n + 2 + 6d - 4p, & \text{if } 1 \leq d \leq \lfloor \frac{p}{4} \rfloor; \\ (p - 2d) + 2(2d + (n + 1 - 2p)) = 2n + 2 + 2d - 3p, & \text{if } \lceil \frac{p}{4} \rceil \leq d \leq \lceil \frac{p}{2} \rceil - 1; \\ 2 \times \frac{p}{2} + (n + 1 - 2p) = n + 1 - p, & \text{if } p \text{ is even and } d = \frac{p}{2}. \end{cases}$$

If $V_r \subseteq V_2$, then $|V_r| = 2$ or 1. Moreover, $|V_r| = 1$ only if n is odd and $d = \frac{n+1-2p}{2}$, and we have $W_{V_r}(r) = n + 1 - 2p - 2d$, where $0 \leq d \leq \lfloor \frac{n+1-2p}{2} \rfloor$.

Next, we will show $GP_a(B_n^{p,p}) \leq GP_a(B_n^{3,3})$ by a direct calculation.

Subcase 1.1. $p = 0(mod\ 4)$.

Then $p \geq 4$. If n is odd, we have

$$\begin{aligned} GP_a(B_n^{p,p}) &= \sum_{d=1}^{\frac{p}{4}}(2n + 2 + 6d - 4p) + \sum_{d=\frac{p+4}{4}}^{\frac{p-2}{2}}(2n + 2 + 2d - 3p) + (n + 1 - p) \\ &\quad + \sum_{d=0}^{\frac{n+1-2p}{2}}(n + 1 - 2p - 2d) \\ &= \frac{n^2}{4} - \frac{3p^2}{8} + p - \frac{1}{4} < \frac{n^2}{4} - \frac{5}{4} \end{aligned}$$

as $p \geq 4$. Similarly, if n is even, then

$$\begin{aligned} GP_a(B_n^{p,p}) &= \sum_{d=1}^{\frac{p}{4}}(2n + 2 + 6d - 4p) + \sum_{d=\frac{p+4}{4}}^{\frac{p-2}{2}}(2n + 2 + 2d - 3p) + (n + 1 - p) \\ &\quad + \sum_{d=0}^{\frac{n-2p}{2}}(n + 1 - 2p - 2d) \\ &= \frac{n^2}{4} - \frac{3p^2}{8} + p < \frac{n^2}{4} - \frac{5}{4} \end{aligned}$$

as $p \geq 4$.

Subcase 1.2. $p = 1(mod\ 4)$.

Then $p \geq 5$. If n is odd, we have

$$\begin{aligned} GP_a(B_n^{p,p}) &= \sum_{d=1}^{\frac{p-1}{4}}(2n+2+6d-4p) + \sum_{d=\frac{p+3}{4}}^{\frac{p-1}{2}}(2n+2+2d-3p) + \sum_{d=0}^{\frac{n+1-2p}{2}}(n+1-2p-2d) \\ &= \frac{n^2}{4} - \frac{3p^2}{8} + p - \frac{7}{8} < \frac{n^2}{4} - \frac{5}{4} \end{aligned}$$

as $p \geq 5$. Similarly, if n is even, then

$$\begin{aligned} GP_a(B_n^{p,p}) &= \sum_{d=1}^{\frac{p-1}{4}}(2n+2+6d-4p) + \sum_{d=\frac{p+3}{4}}^{\frac{p-1}{2}}(2n+2+2d-3p) + \sum_{d=0}^{\frac{n-2p}{2}}(n+1-2p-2d) \\ &= \frac{n^2}{4} - \frac{3p^2}{8} + p - \frac{5}{8} < \frac{n^2}{4} - \frac{5}{4} \end{aligned}$$

as $p \geq 5$.

Subcase 1.3. $p = 2(mod\ 4)$.

Then $p \geq 6$. If n is odd, we have

$$\begin{aligned} GP_a(B_n^{p,p}) &= \sum_{d=1}^{\frac{p-2}{4}}(2n+2+6d-4p) + \sum_{d=\frac{p+2}{4}}^{\frac{p-2}{2}}(2n+2+2d-3p) + (n+1-p) \\ &\quad + \sum_{d=0}^{\frac{n+1-2p}{2}}(n+1-2p-2d) \\ &= \frac{n^2}{4} - \frac{3p^2}{8} + p - \frac{3}{4} < \frac{n^2}{4} - \frac{5}{4} \end{aligned}$$

as $p \geq 6$. Similarly, if n is even, then

$$\begin{aligned} GP_a(B_n^{p,p}) &= \sum_{d=1}^{\frac{p-2}{4}}(2n+2+6d-4p) + \sum_{d=\frac{p+2}{4}}^{\frac{p-2}{2}}(2n+2+2d-3p) + (n+1-p) \\ &\quad + \sum_{d=0}^{\frac{n-2p}{2}}(n+1-2p-2d) \\ &= \frac{n^2}{4} - \frac{3p^2}{8} + p - \frac{1}{2} < \frac{n^2}{4} - \frac{5}{4} \end{aligned}$$

as $p \geq 6$.

Subcase 1.4. $p = 3(mod\ 4)$.

Then $p \geq 3$. If n is odd, we have

$$\begin{aligned} GP_a(B_n^{p,p}) &= \sum_{d=1}^{\frac{p-3}{4}}(2n+2+6d-4p) + \sum_{d=\frac{p+1}{4}}^{\frac{p-1}{2}}(2n+2+2d-3p) + \sum_{d=0}^{\frac{n+1-2p}{2}}(n+1-2p-2d) \\ &= \frac{n^2}{4} - \frac{3p^2}{8} + p - \frac{7}{8} \leq \frac{n^2}{4} - \frac{5}{4} \end{aligned}$$

as $p \geq 3$ and the equality holds only if $p = 3$. Similarly, if n is even, then

$$\begin{aligned} GP_a(B_n^{p,p}) &= \sum_{d=1}^{\frac{p-3}{4}}(2n+2+6d-4p) + \sum_{d=\frac{p+1}{4}}^{\frac{p-1}{2}}(2n+2+2d-3p) + \sum_{d=0}^{\frac{n-2p}{2}}(n+1-2p-2d) \\ &= \frac{n^2}{4} - \frac{3p^2}{8} + p - \frac{5}{8} \leq \frac{n^2}{4} - 1 \end{aligned}$$

as $p \geq 3$ and the equality holds only if $p = 3$.

Case 2. For any $\gamma \in Aut(G)$, $\gamma(V(C_p)) = V(C_p)$.

Let

$$\mathcal{V}_1 = \{x | x \in V(T_w), w \in V(C_p) \setminus \{u\}\},$$

$$\mathcal{V}_2 = \{x | x \in V(T_w), w \in V(C_q) \setminus \{v\}\}$$

and

$$\mathcal{V}_3 = V(G) \setminus (\mathcal{V}_1 \cup \mathcal{V}_2).$$

It can be seen that any orbit of G belongs to $\mathcal{V}_1$, $\mathcal{V}_2$ or $\mathcal{V}_3$. Let $|\mathcal{V}_i| = n_i$ for $1 \leq i \leq 3$. Then $n_1, n_2 \geq 2$ and $n_1 + n_2 + n_3 = n$. Since each $G[\mathcal{V}_i]$ is a tree, by Theorem 2.2, we have

$$GP_a(G[\mathcal{V}_i]) \leq \frac{n_i^2 - 1}{4}$$

for $1 \leq i \leq 3$. Note that some orbits in $\mathcal{V}_i \subseteq V(G)$ may merge into a new orbit of $G[\mathcal{V}_i]$ for $1 \leq i \leq 3$. Hence by Lemma 3.1, we have

$$GP_a(G) \leq \sum_{1 \leq i \leq 3} GP_a(G[\mathcal{V}_i]) \leq \frac{n_1^2 - 1}{4} + \frac{n_2^2 - 1}{4} + \frac{(n - n_1 - n_2)^2 - 1}{4} < \frac{n^2}{4} - \frac{5}{4}$$

as $n_1, n_2 \geq 2$ and $n \geq 5$.

Therefore, we have $GP_a(G) \leq GP_a(B_n^{3,3})$. □

4. Conclusions

In this paper, we consider the Graovac-Pisanski index of ∞-shape bicyclic graphs. Through a series of graph operations, we obtain the maximum Graovac-Pisanski index for all ∞-shaped bicyclic graphs and determine the corresponding extremal graphs. But for the maximum Graovac-Pisanski index of Θ-shape bicyclic graphs, we have not found a good solution, although we conjecture that its maximum value is less than $\frac{n^3}{8} - \frac{n}{2}$.

In addition, for other graph classes such as cactus graphs or even random graphs, we believe that computing the maximum Gravats-Pisansky indices for these graphs are also worthwhile research topics.

Use of AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

The authors declare that they have no conflicts of interest.

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