Unicyclic graphs with the maximal value of Graovac-Pisanski index

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Abstract

Let $G$ be a graph and let $\Gamma$ be its group of automorphisms. Graovac-Pisanski index of $G$ is $\text{GP}(G) = \frac{|V(G)|}{2|\Gamma|} \sum_{u \in V(G)} \sum_{\alpha \in \Gamma} d(u, \alpha(u))$, where $d(u, v)$ is the distance from $u$ to $v$ in $G$. One can observe that $\text{GP}(G) = 0$ if $G$ has no nontrivial automorphisms, but it is not known which graphs attain the maximum value of Graovac-Pisanski index. In this paper we show that among unicyclic graphs on $n$ vertices the $n$-cycle attains the maximum value of Graovac-Pisanski index.

Keywords: Graovac-Pisanski index, modified Wiener index, unicyclic graphs.

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1 Introduction

Wiener index, the sum of distances in a graph, is an important molecular descriptor. It was introduced by Wiener in 1949, see [18], and since then many other molecular descriptor have appeared. One of them is the Graovac-Pisanski index [8], originally known as the modified Wiener index. With this index an algebraic approach for generalizing the Wiener index was presented. Namely, as the Wiener index also the Graovac-Pisanski index is based on distances but its advantage is in considering also the symmetries of a graph, and it is known that symmetries of a molecule have an influence on its properties [14].

In his pioneering paper, Wiener showed a correlation of the Wiener index of alkanes with their boiling points [18]. It turns out that the Graovac-Pisanski index combines the symmetry and topology of molecules to obtain a good correlation with some physico-chemical properties of molecules. Recently, Črepnjak et al. showed that the Graovac-Pisanski index of some hydrocarbon molecules is correlated with their melting points [6].

This index also drew attention from theoretical point of view. Researchers are interested in the difference between the Wiener and Graovac-Pisanski index. This difference was computed in [9] for some families of polyhedral graphs. The Graovac-Pisanski index of nanostructures was studied in [1, 2, 15, 16, 17] and for some classes of fullerenes and fullerene-like molecules in [3, 11, 12]. In [13] the symmetry groups and Graovac-Pisanski index of some linear polymers were computed. Upper and lower bounds for Graovac-Pisanski index were considered in [11]. In [7] and [16] Graovac-Pisanski index was further considered from computational point of view. Exact formulae for the Graovac-Pisanski index for some graph operations are presented in [4]. Recently it was proved that for any connected bipartite graph, as well as for any connected graph on even number of vertices, the Graovac-Pisanski index is an integer number [5].

Let \( G \) be a connected graph. The Graovac-Pisanski index of \( G \) is defined as

\[
GP(G) = \frac{|V(G)|}{2|\text{Aut}(G)|} \sum_{u \in V(G)} \sum_{\alpha \in \text{Aut}(G)} \text{dist}_G(u, \alpha(u)),
\]

where \( \text{Aut}(G) \) is the group of automorphisms of \( G \) and \( \text{dist}_G(u, v) \) denotes the distance from \( u \) to \( v \) in \( G \). However, in the paper we will use a result from [5] to compute this index. To explain the method we need some additional definitions. Let \( G \) be a graph, \( u \in V(G) \) and \( S \subseteq V(G) \). The distance of \( u \) in \( S \), \( w_S(u) \), is defined as

\[
w_S(u) = \sum_{v \in S} \text{dist}_G(u, v).
\]

The group of automorphisms of \( G \) partitions \( V(G) \) into orbits. We say that \( u, v \in V(G) \) belong to the same orbit if there is an automorphism \( \alpha \in \text{Aut}(G) \) such that \( \alpha(u) = v \). Let \( V_1, V_2, \ldots, V_t \) be all the orbits of \( \text{Aut}(G) \) in \( G \). Moreover, for every \( i, 1 \leq i \leq t \), let \( v_i \in V_i \). That is, \( v_i \)'s are the representatives of \( V_i \)'s. It was shown in [5] that

\[
GP(G) = \frac{|V(G)|}{2} \sum_{i=1}^{t} w_{V_i}(v_i). \tag{1.1}
\]

By (1.1), if a graph has no nontrivial automorphisms, that is if all its orbits consist of single vertices, then its Graovac-Pisanski index is 0. Hence, all graphs with no nontrivial automorphisms achieve the minimum value of Graovac-Pisanski index. More interesting is the opposite problem.
Problem 1.1. Find all graphs on $n$ vertices with the maximum value of Graovac-Pisanski index.

This problem was solved for trees in [10]. By a long $H$ on $n$ vertices we denote a tree obtained from a path on $n-4$ vertices by attaching two pendant vertices to each endvertex of the path.

Theorem 1.2. Let $T$ be a tree on $n \geq 8$ vertices with the maximum value of Graovac-Pisanski index. Then $T$ is either a path or a long $H$. Moreover,

$$GP(T) = \begin{cases} \frac{n^3 - n}{2} & \text{if } n \text{ is odd}, \\ \frac{n^3}{4} & \text{if } n \text{ is even}. \end{cases}$$

For $n \leq 7$ there are also three other trees with the maximum value of Graovac-Pisanski index. However, they have the value of Graovac-Pisanski index as stated in Theorem 1.2.

In this paper we prove the following statement.

Theorem 1.3. Let $G$ be a unicyclic graph on $n$ vertices with the maximum value of Graovac-Pisanski index. Then $G$ is the $n$-cycle and

$$GP(C_n) = \begin{cases} \frac{n^3 - n}{2} & \text{if } n \text{ is odd}, \\ \frac{n^3}{4} & \text{if } n \text{ is even}. \end{cases}$$

Observe that Graovac-Pisanski index for extremal trees and for extremal unicyclic graphs has the same value. We believe the following holds.

Conjecture 1.4. Let $G$ be a graph on $n$ vertices, $n \geq 8$, with the maximum value of Graovac-Pisanski index. Then $G$ is either a path, or a long $H$, or a cycle.

To support this conjecture we performed some computer experiments. They showed the validity of the conjecture for $n = 8$ and $n = 9$. We believe that the maximal degree of extremal graphs is small (at most 3), thus for the cases $n = 10$ and $n = 11$ we limited our computer search to maximal degrees 5 and 4, respectively, and in these cases the conjecture was confirmed as well. The graphs from the conjecture are extremal also for $n \in \{5, 6, 7\}$, however when $n$ equals 7 there exists an additional extremal graph.

2 Proof

In this section we prove several claims which imply Theorem 1.3. Obviously, if we consider graphs of order $n$, we do not need to consider the multiplicative term $\frac{n^3}{2}$ in (1.1). Therefore we define

$$GPa(G) = \sum_{i=1}^{t} w_{V_i}(v_i),$$

where $V_1, V_2, \ldots, V_t$ are all the orbits of $Aut(G)$ in $G$ and $v_1, v_2, \ldots, v_t$ are their representatives, respectively. Then for given $n$, graphs on $n$ vertices with the maximum value of $GPa$ are the solutions of Problem 1.1.

For a cycle on $n$ vertices, $GPa(C_n) = w_{V}(v)$ where $v$ is an arbitrary vertex of $C_n$ and $V = V(C_n)$. This implies the following statement.
**Proposition 2.1.** We have

\[
\text{GPa}(C_n) = \begin{cases} 
\frac{n^2-1}{4} & \text{if } n \text{ is odd}, \\
\frac{n^2}{4} & \text{if } n \text{ is even}.
\end{cases}
\]

In what follows we generalize the GPa-parameter. Let \( Z = \{Z_1, \ldots, Z_t\} \) be a partition of \( V(G) \) and let \( z_i \in Z_i, 1 \leq i \leq t \). Then

\[
\text{GPa}^Z(G) = \sum_{i=1}^{t} w_{Z_i}(z_i).
\]

In our proofs, sets \( Z_i \) will usually be unions of orbits of \( \text{Aut}(G) \). Nevertheless, \( \text{GPa}^Z(G) \) will depend on the choice of the representatives \( z_i \).

To prove Theorem 1.3 we start with \( \text{GPa}(G) \), where \( G \) is an extremal unicyclic graph on \( n \) vertices different from the \( n \)-cycle. Then in a sequence of steps we modify either the graph or the partition and in each step we obtain a larger value of \( \text{GPa}^Z \). Since we terminate this process with \( C_n \) and \( \text{GPa} \), we get the result.

Hence, let \( G \) be a unicyclic graph on \( n \) vertices with the maximum value of Graovac-Pisanski index and such that \( G \) is not the \( n \)-cycle. Then \( G \) consists of a single cycle \( C \) and trees rooted at the vertices of the cycle. In what follows, orbits of vertices of \( C \) will be important.

We start with modifying the partition by merging together some orbits of vertices which have the same distance from \( C \). We denote by \( \mathcal{X} \) the new partition of \( V(G) \), while the original partition into orbits is denoted by \( \mathcal{Y} \). Let \( v \) be a vertex of \( C \). If \( \{v\} \) is a trivial orbit of \( \text{Aut}(G) \), then orbits in the \( v \)-rooted tree form sets of the partition \( \mathcal{X} \). But if \( \{v\} \) is not a trivial orbit of \( \text{Aut}(G) \), we do the following. Let \( O_v \) be the orbit of \( \text{Aut}(G) \) containing \( v \) and let \( O_v(G) \) be the set of vertices of \( u \)-rooted trees where \( u \in O_v \). We partition the vertices of \( O_v(G) \) according to their distance from \( C \). Hence, \( O_v \) alone is one set of \( \mathcal{X} \), another set of \( \mathcal{X} \) contains those vertices of \( O_v(G) \) which are adjacent to a vertex of \( C \), etc.

We have the following statement.

**Lemma 2.2.** For arbitrary choice of the representatives of sets in \( \mathcal{X} \) we have

\[
\text{GPa}(G) \leq \text{GPa}^\mathcal{X}(G).
\]

**Proof.** Let \( X_i \) be a set from \( \mathcal{X} \) and let \( x_i \) be an arbitrary vertex of \( X_i \). Observe that \( X_i \) is a union of several orbits of \( \text{Aut}(G) \). Let \( V_0 \) be an orbit of \( \text{Aut}(G) \) such that \( V_0 \subseteq X_i \). Then \( w_{V_0}(u) \) is the same for every \( u \in V_0 \). So let \( v_0 \) be a vertex of \( V_0 \) at the shortest distance from \( x_i \). Then both \( x_i \) and \( v_0 \) are in the same tree rooted at a vertex of \( C \). Assume that they are in a \( v \)-rooted tree \( T \).

Let \( u \) be a vertex of \( V_0 \). If \( u \) is not in \( T \) then \( \text{dist}_G(x_i, u) = \text{dist}_G(v_0, u) \) since \( \text{dist}_G(x_i, v) = \text{dist}_G(v_0, v) \). So let \( u \) be a vertex in \( T \). Let \( z \) be a vertex on the (unique) \((v_0, u)\)-path at the shortest distance from \( v \). Since \( v_0 \) is a vertex of \( V_0 \) at the shortest distance from \( x_i \), the shortest \((x_i, u)\)-path must contain \( z \). Thus \( \text{dist}_G(v_0, u) \leq \text{dist}_G(x_i, u) \) and so \( w_{V_0}(v_0) \leq w_{V_0}(x_i) \). Consequently, \( \text{GPa}(G) \leq \text{GPa}^\mathcal{X}(G) \) as required.

Now we modify the graph \( G \), and we consider a partition \( \mathcal{Y} \) of the vertex set of the modified graph inherited from the partition \( \mathcal{X} \) of \( G \). So let \( v \) be a vertex of \( C \). If \( \{v\} \) is a
trivial orbit of $\text{Aut}(G)$ then we do not change the $v$-rooted tree, and its orbits form sets of the partition $\mathcal{Y}$. Hence, in this case the sets of $\mathcal{Y}$ coincide with the sets of $\mathcal{X}$ (and also with the orbits of $V$). But if $\{v\}$ is not a trivial orbit of $\text{Aut}(G)$ then we change the $v$-rooted tree. If the $v$-rooted tree has $p$ vertices in $G$ then we replace it by a path on $p$ vertices rooted at the endvertex, which we again denote by $v$. Denote by $F$ the graph which results when all these replacements are made. Since we did not change the cycle, we denote the cycle of $F$ again by $C$. Let $O_v$ be the orbit of $\text{Aut}(G)$ containing $v$. By our assumption $|O_v| \geq 2$.

Analogously as above, let $O_u(F)$ be the set of vertices of $u$-rooted trees where $u \in O_v$. Partition $O_u(F)$ into $p$ disjoint sets of $\mathcal{Y}$ according to their distance from $C$.

Observe that for every $Y_i \in \mathcal{Y}$ and for every two vertices $y_i^1, y_i^2 \in Y_i$ we have $w_{Y_i}(y_i^1) = w_{Y_i}(y_i^2)$. Hence when computing $\text{GPa}^{\mathcal{Y}}(F)$, we can choose the representatives $y_i$ in $Y_i$ arbitrarily. However, orbits of $F$ may be strictly larger than the sets $Y_i$. This is caused by the fact that two non-isomorphic rooted trees may have the same numbers of vertices. Our next statement follows.

**Lemma 2.3.** For arbitrary choice of representatives of sets in $\mathcal{Y}$ we have

$$\text{GPa}^{\mathcal{X}}(G) \leq \text{GPa}^{\mathcal{Y}}(F).$$

**Proof.** Let $H$ be a graph. A ray in $H$ is a subgraph of $H$ which is isomorphic to a path, its first vertex has degree at least 3 in $H$, its last vertex has degree 1 in $H$ and all the other vertices have degree 2 in $H$.

We do not prove the inequality directly. Instead, we construct a sequence of graphs $G = G^0, G^1, \ldots, G^q = F$, each $G^i$ with a partition $\mathcal{X}^i$, such that

$$\text{GPa}^{\mathcal{X}^i}(G^i) \leq \text{GPa}^{\mathcal{X}^{i+1}}(G^{i+1})$$

for a special choice of representatives in $\mathcal{X}^{i+1}$, where $0 \leq i < q$, $\mathcal{X}^0 = \mathcal{X}$ and $\mathcal{X}^q = \mathcal{Y}$. We remark that for every $i$, $G^i$ will be a unicyclic graph with the cycle $C$ such that if $O = \{v_1, \ldots, v_t\}$ is an orbit of vertices of $C$ in $G$, then all $v_j$-rooted trees in $G^i$ are mutually isomorphic, $1 \leq j \leq t$. If $t = 1$ then the $v_1$-rooted trees in $G, G^1, \ldots, F$ are mutually isomorphic and all $\mathcal{X}, \mathcal{X}^1, \ldots, \mathcal{Y}$ coincide on the vertex sets of these trees. However if $t \geq 2$, then the vertex set $O_{v_1}(G^i)$ of the $v_1$-rooted trees, $1 \leq j \leq t$, is partitioned in $\mathcal{X}^i$ according to the distance from $C$, and we assume that all the representatives of these sets are in the $v_1$-rooted tree. This assumption is possible since $O$ is an orbit in $G$, and although $O$ does not need to be an orbit of $G^i$, the vertices of $O$ are nicely distributed along the cycle $C$ in $G^i$.

So consider $i$, $0 \leq i < q$. We assume that $G^i$ is already known and we construct $G^{i+1}$. For this, let $O = \{v_1, \ldots, v_t\}$ be an orbit of vertices of $C$ in $G$, where $t \geq 2$. If the $v_1$-rooted tree (and so also $v_j$-rooted trees for $2 \leq j \leq t$) is a path rooted at the endvertex, then we are done with this orbit of $G$. So suppose that the $v_1$-rooted tree has at least two endvertices different from $v_1$, and consequently, at least two distinct rays starting at a common vertex. Let $R_1$ and $R_2$ be two rays starting at a vertex $c$ such that $\text{dist}_{G^i}(v_1, c)$ is maximum possible. We assume that $R_1$ is not shorter than $R_2$. If there is a representative $x_j^i$ of $X_j^i$ which is in $R_2$, then replace it by a vertex of $X_j^i$ in $R_1$. Observe that this replacement does not change $\text{GPa}^{\mathcal{X}^i}(G^i)$. Now delete $R_2$ from the $v_1$-rooted tree and attach it to the second vertex of $R_1$. Moreover, repeat the same procedure in all the other $v_j$-rooted trees, $2 \leq j \leq t$, and denote by $G^{i+1}$ the resulting graph. Denote by $T^i$ and $T^{i+1}$ the $v_1$-rooted
tree in $G^i$ and $G^{i+1}$, respectively. If $R_1$ and $R_2$ have the same length, then this operation may create a new set in $X^{i+1}$, because $T^i$ may have smaller depth than $T^{i+1}$ (As is the custom, by depth we denote the largest distance from the root.) In such a case choose a representative of this new set in $R_2$. This is the unique case when a representative will be in $R_2$ in $T^{i+1}$.

Let $d = \text{dist}_{G^i}(v_1, c)$ and let $\ell$ be the length of $R_2$. Assume that the indices of sets in $X^i$ and $X^{i+1}$ are chosen so that $X^i_{j+1}$ in $G^{i+1}$ was obtained from $X^i_j$ in $G^i$ and the representatives of $X^i_j$ and $X^{i+1}_j$ coincide whenever possible. Then $w_{X^i_j}(x^i_j)$ in $G^i$ may differ from $w_{X^{i+1}_j}(x^{i+1}_j)$ in $G^{i+1}$ only if $X^{i+1}_j$ contains vertices of $v_k$-rooted trees, $1 \leq k \leq t$, which are at distance $d + 1$, $d + 2$, $\ldots$, $d + \ell + 1$ from $C$. We distinguish three cases.

**Case 1:** $X^{i+1}_j$ contains vertices at distance $d + 1$ from $C$. Then in the $v_1$-rooted tree, $X^{i+1}_j$ is smaller than $X^i_j$ by exactly one vertex. Consequently $|X^i_j| - |X^{i+1}_j| = t$. Comparing to $\text{GPa}^X_i(G^i)$, $\text{GPa}^{X^{i+1}}_i(G^{i+1})$ is decreased by 2 due to a missing vertex in $T^{i+1}$ and it is decreased by $(t - 1)2(d + 1) + c$ due to missing vertices in $v_k$-rooted trees $2 \leq k \leq t$. Here $c$ represents the distances using the edges of $C$, that is $c = \sum_{k=2}^t \text{dist}_{G}(v_1, v_k)$. Hence,

$$w_{X^{i+1}_j}(x^{i+1}_j) - w_{X^i_j}(x^i_j) = -2 - (t - 1)2(d + 1) - c. \quad (2.2)$$

**Case 2:** $X^{i+1}_j$ contains vertices at distance $d + a$ from $C$, where $2 \leq a \leq \ell$. Then $|X^{i+1}_j| = |X^i_j|$ and comparing to $\text{GPa}^X_i(G^i)$, $\text{GPa}^{X^{i+1}}_i(G^{i+1})$, is decreased by 2 due to a shorter distance to a vertex of $X^{i+1}_j$ in $R_2$. Hence,

$$w_{X^{i+1}_j}(x^{i+1}_j) - w_{X^i_j}(x^i_j) = -2. \quad (2.3)$$

**Case 3:** $X^{i+1}_j$ contains vertices at distance $d + \ell + 1$ from $C$. Then in the $v_1$-rooted tree, $X^{i+1}_j$ is larger than $X^i_j$ by exactly one vertex. Consequently $|X^i_j| - |X^{i+1}_j| = t$. Comparing to $\text{GPa}^X_i(G^i)$, $\text{GPa}^{X^{i+1}}_i(G^{i+1})$ is increased by $(t - 1)2(d + \ell + 1) + c$ due to new vertices in $v_k$-rooted trees, $2 \leq k \leq t$. Here $c$ is the very same constant as in Case 1, that is $c = \sum_{k=2}^t \text{dist}_{G}(v_1, v_k)$. In some cases, namely if $X^i_j$ is not empty, $\text{GPa}^X_i$ is increased by at least 2 due to a new vertex in $T^{i+1}$, but we do not need to consider this contribution in our calculations. Hence,

$$w_{X^{i+1}_j}(x^{i+1}_j) - w_{X^i_j}(x^i_j) \geq (t - 1)2(d + \ell + 1) + c. \quad (2.4)$$

Since $w_{X^{i+1}_j}(x^{i+1}_j) = w_{X^i_j}(x^i_j)$ when $X^i_j \not\subseteq O_{v_i}(G^i)$, summing the expressions (2.2), (2.3) and (2.4) we get

$$\text{GPa}^{X^{i+1}}_i(G^{i+1}) - \text{GPa}^X_i(G^i) \geq (-2 - (t - 1)2(d + 1) - c) - (\ell - 1)2$$

$$+ ((t - 1)2(d + \ell + 1) + c)$$

$$= (t - 2)2\ell \geq 0$$

since $t \geq 2$. \(\square\)

Let $Y_i \in \mathcal{Y}$. Observe that if $Y_i \cap V(C) \neq \emptyset$, then $Y_i \subseteq V(C)$. Let $\mathcal{Y}'$ be those sets of $\mathcal{Y}$ which contain vertices of $V(C)$. We define a new partition $\mathcal{Z}$ of $F$ as follows:

$$\mathcal{Z} = \mathcal{Y} \setminus \mathcal{Y}' \cup V(C).$$
That is, we merge together all sets \( Y_i \) containing vertices of \( V(C) \). All the other sets of \( Z \) coincide with the sets of \( \mathcal{Y} \). We have the following statement.

**Lemma 2.4.** For arbitrary choice of representatives of sets in \( Z \) we have

\[
\text{GPa}^\mathcal{Y}(F) \leq \text{GPa}^Z(F).
\]

**Proof.** Observe that there are three types of sets in \( Z \). First, if \( v_1 \in V(C) \) is a trivial orbit in \( G \), then orbits of vertices of the \( v_1 \)-rooted tree are sets of \( Z \). Second, if \( \{v_1, \ldots, v_\ell\} \subseteq V(C) \) is a non-trivial orbit in \( G \), that is if \( \ell \geq 2 \), then the \( v_1 \)-rooted trees are paths with endvertices \( v_i \), and sets of vertices of \( O_{v_1}(F) \) in \( Z \) contain vertices of these \( \ell \) root trees which are at the same distance from \( C \). Finally, \( Z \) contains \( V(C) \). If \( Z_i \) is a set of \( Z \) of the first type or of the second type and \( u, v \in Z_i \), then \( w_{Z_i}(u) = w_{Z_i}(v) \). Hence, to prove the statement it suffices to show that

\[
\sum_{Y_i \in \mathcal{Y}'} w_{Y_i}(y) \leq w_{V(C)}(z) = \sum_{Y_i \in \mathcal{Y}'} w_{Y_i}(z)
\]

where \( z \) is an arbitrary vertex of \( V(C) \) and \( \mathcal{Y}' \) is defined before Lemma 2.4. (Recall that \( y_i \) is a representative of \( Y_i \) in \( \mathcal{Y} \).

Thus, let \( z \in V(C) \) and let \( Y_i \in \mathcal{Y}' \). In what follows we show that \( w_{Y_i}(y_i) \leq w_{Y_i}(z) \). We distinguish four cases.

**Case 1:** \( |Y_i| = 1 \). Since \( w_{Y_i}(y_i) = 0 \leq \text{dist}_F(z, y_i) = w_{Y_i}(z) \), we have \( w_{Y_i}(y_i) \leq w_{Y_i}(z) \).

**Case 2:** \( |Y_i| = 2 \). Let \( Y_i = \{y_i, y\} \). Then by triangle inequality

\[
w_{Y_i}(y) = \text{dist}_F(z, y) \leq \text{dist}_F(z, y_i) + \text{dist}_F(y, z) = w_{Y_i}(z).
\]

Hence, in the sequel we assume that \( |Y_i| \geq 3 \). Since \( Y_i \) is an orbit of vertices of \( C \) in \( G \), there is a nontrivial rotational automorphism \( \alpha \) in Aut(\( G \)) such that \( \{\alpha^k(y_i) \mid k \in \mathbb{N}\} \subseteq Y_i \). Let \( r \) be the biggest order of a rotational automorphism of this type and let \( \alpha \) be the corresponding automorphism. Observe that \( r \geq 2 \). Since \( w_{Y_i}(u) = w_{Y_i}(v) \) for \( u, v \in Y_i \), we assume that \( y_i \) is chosen so that \( \text{dist}_F(z, y_i) \) is smallest possible.

**Case 3:** \( r \) is even. Let \( Y_i' = \{\alpha^k(y_i) \mid 0 \leq k < r\} \). We rename vertices of \( Y_i' \) as \( \{y^0, y^1, \ldots, y^{r-1}\} \) so that \( \text{dist}_F(y_i, y^k) \leq \text{dist}_F(y_i, y^{k+1}) \) whenever \( 0 \leq k < r - 1 \). Observe that \( y^0 = y_i \), the vertices \( y^{2\ell-1} \) and \( y^{2\ell} \) have the same distance from \( y_i \) if \( 1 \leq \ell < r/2 \) and \( y^{r-1} \) is the unique vertex of \( Y_i' \) with the largest distance from \( y_i \). Since \( y_i \) is the vertex of \( Y_i \) with the smallest distance from \( z \), we have

\[
\text{dist}_F(y^{2\ell-1}, y_i) + \text{dist}_F(y_i, y^{2\ell}) = \text{dist}_F(y^{2\ell-1}, z) + \text{dist}_F(z, y^{2\ell})
\]

for \( 1 \leq \ell < r/2 \) and also

\[
\text{dist}_F(y_i, y^{r-1}) = \text{dist}_F(y_i, z) + \text{dist}_F(z, y^{r-1}) = \frac{1}{2}|V(C)|.
\]

Hence, \( w_{Y_i'}(y_i) = w_{Y_i'}(z) \). If \( Y_i = Y_i' \), we are done. Therefore, in the sequel assume that there is also a reflectin \( \beta \) such that \( \beta(Y_i') \subseteq Y_i \) and \( \beta(Y_i') \cap Y_i' = \emptyset \). Then \( Y_i = Y_i' \cup \beta(Y_i') \) and \( |Y_i| = 2r \). Observe that all the vertices of \( \beta(Y_i') \) are obtained from arbitrary one of
them using $\alpha$. Thus, let $y_i^\beta$ be a vertex of $\beta(Y'_i)$ with the smallest distance from $y_i$. Then using the same arguments as above we get

$$w_{\beta(Y'_i)}(y_i^\beta) = w_{\beta(Y'_i)}(y_i).$$

Since $w_{\beta(Y'_i)}(y_i^\beta) = w_{Y'_i}(y_i)$, we get

$$w_{Y'_i}(y_i) = 2w_{Y'_i}(y_i).$$

Analogously as in Lemma 2.3, we prove the statement by a sequence of steps. Let $y_i^\beta$ be a vertex of $\beta(Y'_i)$ at the smallest distance from $z$, we get

$$w_{\beta(Y'_i)}(y_i^\beta) = w_{\beta(Y'_i)}(z).$$

Since $w_{\beta(Y'_i)}(y_i^\beta) = w_{Y'_i}(y_i)$, we obtain $w_{Y'_i}(y_i) = w_{Y'_i}(z)$.

**Case 4: $r$ is odd.** Let $Y'_i = \{\alpha^k(y_i) \mid 0 \leq k < r\}$. Then proceeding analogously as in Case 3 one gets

$$w_{Y'_i}(z) = w_{Y'_i}(y_i) + \text{dist}_F(y_i, z),$$

and so $w_{Y'_i}(y_i) \leq w_{Y'_i}(z)$ if $Y'_i = Y'_i$. Hence, assume that there is a reflexion $\beta$ such that $\beta(Y'_i) \subseteq Y_i$ and $\beta(Y'_i) \cap Y'_i = \emptyset$. Again, $Y_i = Y'_i \cup \beta(Y'_i)$ and $|Y_i| = 2r$, and all the vertices of $\beta(Y'_i)$ are obtained from arbitrary one of them using $\alpha$. Thus, let $y_i^\beta$ be a vertex of $\beta(Y'_i)$ with the shortest distance from $y_i$. Then analogously as in Case 3 one gets

$$w_{Y'_i}(y_i) = w_{\beta(Y'_i)}(y_i^\beta) = w_{\beta(Y'_i)}(y_i) - \text{dist}_F(y_i^\beta, y_i)$$

and so

$$w_{Y'_i}(y_i) = 2w_{Y'_i}(y_i) + \text{dist}_F(y_i^\beta, y_i).$$

Also, let $y_i^\beta$ be a vertex of $\beta(Y'_i)$ with the smallest distance from $z$. Then analogously as above we get

$$w_{Y'_i}(y_i) = w_{\beta(Y'_i)}(y_i^\beta) = w_{\beta(Y'_i)}(z) - \text{dist}_F(y_i^\beta, z)$$

and so

$$w_{Y'_i}(z) = 2w_{Y'_i}(y_i) + \text{dist}_F(y_i^\beta, z) + \text{dist}_F(y_i, z).$$

Since

$$\text{dist}_F(y_i^\beta, y_i) \leq \text{dist}_F(y_i^\beta, y_i) \leq \text{dist}_F(y_i^\beta, z) + \text{dist}_F(y_i, z),$$

we get $w_{Y'_i}(y_i) \leq w_{Y'_i}(z)$. 

Finally, we are in a position to prove the last lemma which implies Theorem 1.3. Observe that there is a strict inequality in Lemma 2.5.

**Lemma 2.5.** We have

$$\text{GPa}^2(F) < \text{GPa}(C_n).$$

**Proof.** Analogously as in Lemma 2.3, we prove the statement by a sequence of steps. Let $O^1, \ldots, O^q$ be all orbits of vertices of $C$ in $G$, such that for every $v \in O^i$ the $v$-rooted tree is nontrivial (i.e., it has more than one vertex). Observe that if the $v$-rooted tree is nontrivial in $G$, then the $v$-rooted tree in $F$ is also nontrivial. Assume that $|O^1| \geq |O^2| \geq \cdots \geq |O^q|$. 

We consecutively create unicyclic graphs $F = F^0, F^1, \ldots, F^q = C_n$ with partitions $Z = Z^0, Z^1, \ldots, Z^q$, respectively, and for every $i$, $0 \leq i < q$, we show that $GPa_{Z^i}(F^i) < GPa_{Z^{i+1}}(F^{i+1})$. The graph $F^{i+1}$ is obtained from $F^i$ by moving the vertices of $v$-rooted trees, where $v \in O^{i+1}$, into the unique cycle $C^i$ of $F^i$. Now we describe the process in detail.

Choose $i$, $0 \leq i < q$. For $v \in O^{i+1}$, let $p + 1$ be the number of vertices of $v$-rooted tree in $F^i$ (or in $G$, since the numbers of vertices of $v$-rooted trees in $G$ and $F$ are the same). By our assumption $p \geq 1$. Orient the cycle $C^i$ of $F^i$ and for every vertex $u \in V(C^i)$ let $u^f$ be the vertex following $u$ on $C^i$. Let $v \in O^{i+1}$. Delete the $p$ non-root vertices of the $v$-rooted tree from $F^i$ and subdivide the edge $vv^f$ exactly $p$ times. Repeat this procedure for all vertices of $O^{i+1}$ and denote by $F^{i+1}$ the resulting unicyclic graph. The partition $Z^{i+1}$ is exactly the same as $Z^i$, the only exception is that instead of the set $V(C^i)$ and various sets partitioning $O_v(F^i)$ for $v \in O^{i+1}$ we have just the set $V(C^{i+1})$ in $Z^{i+1}$. We assume that if a set of $Z^i$ is identical with a set of $Z^{i+1}$, then they have the same representatives.

Let $Z' \in Z^i$ and $Z^* \in Z^{i+1}$ such that $Z' = Z^*$. Then $Z'$ is a collection of vertices of $O_a(F^i)$, i.e., of $u$-rooted trees for $u \in O^j$, where $j > i + 1$. Since the distances between these vertices cannot be shorter in $F^{i+1}$ than in $F^i$ (they can be only larger due to the extension of $C^i$ to $C^{i+1}$), we have $w_{Z'}(z') \leq w_{Z^*}(z^*)$ where $z'$ is a representative of $Z'$ in $F^i$ and $z^*$ is a representative of $Z^*$ in $F^{i+1}$. Hence, it suffices to check the contribution of $V(C^{i+1})$ in $GPa_{Z^{i+1}}(F^{i+1})$ and in $GPa_{Z^i}(F^i)$ the contribution of $V(C^i)$ and of the sets of non-root vertices of $v$-rooted trees for $v \in O^{i+1}$. Let $t = |O^{i+1}|$. Analogously as in the proof of Lemma 2.4 we distinguish four cases. In these cases, we set $c = |V(C^i)|$. Moreover, by $\delta_a$ we denote the parity of $a$. That is $\delta_a = 1$ if $a$ is odd and $\delta_a = 0$ if $a$ is even.

**Case 1:** $t = 1$. By Proposition 2.1, $V(C^i)$ contributes $\frac{1}{4}(c^2 - \delta_c)$ to $GPa_{Z^i}(F^i)$ and $V(C^{i+1})$ contributes $\frac{1}{4}((c + p)^2 - \delta_{c+p})$ to $GPa_{Z^{i+1}}(F^{i+1})$. Let $O^{i+1} = \{v_1\}$. Denote by $T$ the $v_1$-rooted tree in $F^i$. Since $T$ is a tree on $p + 1$ vertices, the orbits of $T$ contribute to $GPa_{Z^i}(F^i)$ at most $\frac{1}{4}((p + 1)^2 - \delta_{p+1})$ by Theorem 1.2. So

$$4(GPa_{Z^{i+1}}(F^{i+1}) - GPa_{Z^i}(F^i)) \geq (c + p)^2 - \delta_{c+p} - c^2 + \delta_c - (p + 1)^2 + \delta_{p+1}$$

$$\geq (c + p)^2 - c^2 - (p + 1)^2 - 1$$

$$= 2p(c - 1) - 2 > 0$$

since $c \geq 3$ and $p \geq 1$.

**Case 2:** $t = 2$. In this case the $v$-rooted trees are paths whenever $v \in O^{i+1}$. Since the contribution to $GPa_{Z^i}(F^i)$ of $j$-th vertices of these paths (i.e., of vertices at distance $j$ from the roots) is at most $j + c/2 + j$, the total contribution of non-root vertices of $v$-rooted trees, $v \in O^{i+1}$, is at most $2(p+1) + \frac{1}{2}cp$. Since the contribution of $V(C^i)$ is $\frac{1}{4}(c^2 - \delta_c)$ and the contribution of $V(C^{i+1})$ is $\frac{1}{4}((c + 2p)^2 - \delta_{c+2p})$, where $\delta_{c+2p} = \delta_c$, we get

$$4(GPa_{Z^{i+1}}(F^{i+1}) - GPa_{Z^i}(F^i)) \geq (c + 2p)^2 - \delta_c - c^2 + \delta_c - 8\left(p^2/2\right) - 2cp$$

$$\geq (c + 2p)^2 - c^2 - 4p^2 - 4p - 2cp$$

$$= 2p(c - 2) > 0$$

since $c \geq 3$ and $p \geq 1$.
In the remaining cases we may assume that there is a nontrivial rotational automorphism \( \alpha \) of \( F^i \) such that when \( v \in O^{i+1} \) then also \( \alpha(v) \in O^{i+1} \). Let \( r \) be the biggest order of such a rotational automorphism \( \alpha \), and moreover, let \( \beta \) be such that the distance \( s \) between \( v \) and \( \alpha(v) \) is the smallest possible. Then \( c = r \cdot s \).

**Case 3:** \( r \) is even. Then \( r \geq 2 \). Let \( v_0 \in O^{i+1} \). Denote \( O' = \{ \alpha^k(v_0) \mid 0 \leq k < r \} \). First assume that \( |O^{i+1}| = 2r \). Hence there is also a reflexion \( \beta \) such that \( \beta(O') \subseteq O^{i+1} \) and \( \beta(O') \cap O' = \emptyset \). Let \( v_1 \in O^{i+1} \) such that the distance \( t \) between \( v_0 \) and \( v_1 \) is the smallest possible. Then \( t \leq s/2 \) and \( v_1 \in \beta(O') \). Observe that now \( t \geq 1 \) and \( s \geq 2 \). Since \( c = rs \) is even, the contribution of \( V(C^i) \) to \( \text{GPa}^{Z^i}(F^i) \) is \( \frac{1}{4} r^2 s^2 \). The contribution of \( V(C^{i+1}) \) to \( \text{GPa}^{Z^{i+1}}(F^{i+1}) \) is \( \frac{1}{4} r^2 (s+2p)^2 \). Now we calculate the contribution of non-root vertices of \( v \)-rooted trees when \( v \in O^{i+1} \). These trees are paths and the contribution of \( j \)-th vertices is

\[
2(s+2j) + 2(2s+2j) + \cdots + 2\left(\left(\frac{r}{2} - 1\right) s + 2j\right) + \left(\frac{s}{2} s + 2j\right) \\
+ (t+2j) + (s+t+2j) + \cdots + \left(\left(\frac{r}{2} - 1\right) s + t + 2j\right) + (s-t+2j) \\
+ (2s-t+2j) + \cdots + \left(\left(\frac{r}{2} - 1\right) s - t + 2j\right) + \left(\frac{s}{2} s - t + 2j\right) \\
= 4(s+2j) + 4(2s+2j) + \cdots + 4\left(\left(\frac{r}{2} - 1\right) s + 2j\right) + 2\left(\frac{s}{2} s + 2j\right) + 2j \\
= \frac{1}{2} r^2 s + 2j(2r-1).
\]

So the contribution of non-root vertices of \( v \)-rooted trees, \( v \in O^{i+1} \), is

\[
\sum_{j=1}^{p} \left(\frac{1}{2} r^2 s + 2j(2r-1)\right) = \frac{1}{2} r^2 s p + (p^2 + p)(2r - 1).
\]

Hence

\[
\text{GPa}^{Z^{i+1}}(F^{i+1}) - \text{GPa}^{Z^i}(F^i) \geq \frac{1}{4} r^2 s^2 + r^2 s p + r^2 p^2 - \frac{1}{4} r^2 s^2 - \frac{1}{2} r^2 s p - 2rp^2 - 2rp + p^2 + p \\
= p^2(r-1)^2 + p(r\left(\frac{1}{2} rs - 2\right) + 1) > 0
\]

since \( r \geq 2 \), \( s \geq 2 \) and \( p \geq 1 \).

In the case when \( |O^{i+1}| = r \), the contribution of \( V(C^{i+1}) \) is \( \frac{1}{4} r^2 (s+p)^2 \) and the contribution of \( j \)-th vertices in \( v \)-rooted trees, \( v \in O^{i+1} \), is

\[
2(s+2j) + 2(2s+2j) + \cdots + 2\left(\left(\frac{r}{2} - 1\right) s + 2j\right) + \left(\frac{s}{2} s + 2j\right) = \frac{1}{4} r^2 s + 2j(r-1).
\]

So the contribution of non-root vertices of \( v \)-rooted trees, \( v \in O^{i+1} \), is

\[
\sum_{j=1}^{p} \left(\frac{1}{4} r^2 s + 2j(r-1)\right) = \frac{1}{4} r^2 s p + (p^2 + p)(r - 1).
\]

Hence

\[
\text{GPa}^{Z^{i+1}}(F^{i+1}) - \text{GPa}^{Z^i}(F^i) \geq \frac{1}{4} r^2 s^2 + \frac{1}{2} r^2 s p + \frac{1}{4} r^2 p^2 - \frac{1}{4} r^2 s^2 - \frac{1}{4} r^2 s p - rp^2 - rp + p^2 + p \\
= p^2\left(\frac{r}{2} - 1\right)^2 + p(r\left(\frac{1}{4} rs - 1\right) + 1) > 0
\]
since in this case \( r \geq 4, s \geq 1 \) and \( p \geq 1 \).

**Case 4:** \( r \) is odd. Then \( r \geq 3 \). Let \( v_0 \in O^{i+1} \) and \( O' = \{ \alpha^k(v_0) \mid 0 \leq k < r \} \). First assume that \( |O^{i+1}| = 2r \). Hence there is also a reflexion \( \beta \) such that \( \beta(O') \subseteq O^{i+1} \) and \( \beta(O') \cap O' = \emptyset \). Let \( v_1 \in O^{i+1} \) such that the distance \( t \) between \( v_0 \) and \( v_1 \) is the smallest possible. Then \( t \leq s/2 \) and \( v_1 \in \beta(O') \). The contribution of \( V(C^i) \) to \( \text{GPa}^{Z^i}(F^i) \) is \( \frac{1}{4}(r^2 s^2 - \delta_{rs}) \). The contribution of \( V(C^{i+1}) \) to \( \text{GPa}^{Z^{i+1}}(F^{i+1}) \) is \( \frac{1}{4}(r^2 s + 2p)^2 - \delta_{r(s+2p)} \). Now we calculate the contribution of non-root vertices of \( v \)-rooted trees when \( v \in O^{i+1} \). These trees are paths and the contribution of \( j \)-th vertices is

\[
2(s + 2j) + 2(2s + 2j) + \cdots + 2\left(\frac{r-1}{2}s + 2j\right) \\
+ (t + 2j) + (s + t + 2j) + \cdots + \left(\frac{r-1}{2}s + t + 2j\right) \\
+ (s - t + 2j) + (2s - t + 2j) + \cdots + \left(\frac{r-1}{2}s - t + 2j\right) \\
= 4(s + 2j) + 4(2s + 2j) + \cdots + 4\left(\frac{r-1}{2}s + 2j\right) + (t + 2j) \\
= \frac{1}{2}(r^2 - 1)s + 2j(2r - 1) + t.
\]

So the contribution of non-root vertices of \( v \)-rooted trees, \( v \in O^{i+1} \), is

\[
\sum_{j=1}^{p} \left(\frac{1}{2}(r^2 - 1)s + 2j(2r - 1) + t\right) = \frac{1}{2}(r^2 - 1)s + (p^2 + p)(2r - 1) + pt \\
\leq \frac{1}{2}r^2sp + (p^2 + p)(2r - 1)
\]

since \( -\frac{1}{2}sp + pt \leq 0 \). Hence

\[
\text{GPa}^{Z^{i+1}}(F^{i+1}) - \text{GPa}^{Z^i}(F^i) \geq \frac{1}{4}r^2 s^2 + r^2 sp + r^2 p^2 - \frac{1}{4}\delta_{rs} - \frac{1}{4}r^2 s^2 + \frac{1}{4}\delta_{rs} \\
- \frac{1}{4}r^2 sp - 2rp^2 - 2rp + p^2 + p \\
= p^2(r - 1)^2 + p(r\left(\frac{1}{2}rs - 2\right) + 1) > 0
\]

since \( r \geq 3, s \geq 2 \) and \( p \geq 1 \).

In the case when \( |O^{i+1}| = r \), the contribution of \( V(C^{i+1}) \) to \( \text{GPa}^{Z^{i+1}}(F^{i+1}) \) is \( \frac{1}{4}(r^2(s + p))^2 - \delta_{r(s+p)} \) and the contribution of \( j \)-th vertices in \( v \)-rooted trees, \( v \in O^{i+1} \), is

\[
2(s + 2j) + 2(2s + 2j) + \cdots + 2\left(\frac{r-1}{2}s + 2j\right) = \frac{1}{4}(r^2 - 1)s + 2j(r - 1).
\]

So the contribution of non-root vertices of \( v \)-rooted trees, \( v \in O^{i+1} \), is

\[
\sum_{j=1}^{p} \left(\frac{1}{4}(r^2 - 1)s + 2j(r - 1)\right) = \frac{1}{4}(r^2 - 1)sp + (p^2 + p)(r - 1).
\]

Hence

\[
\text{GPa}^{Z^{i+1}}(F^{i+1}) - \text{GPa}^{Z^i}(F^i) \geq \frac{1}{4}r^2 s^2 + \frac{1}{2}r^2 sp + \frac{1}{4}r^2 p^2 - \frac{1}{4} - \frac{1}{4}r^2 s^2 \\
- \frac{1}{4}(r^2 - 1)sp - rp^2 - rp + p^2 + p \\
= p^2\left(\frac{1}{2} - 1\right)^2 + p(r\left(\frac{1}{2}rs - 1\right) + \frac{1}{2}s + 1) - \frac{1}{4} > 0
\]

since in this case \( r \geq 3, s \geq 1 \) and \( p \geq 1 \). (Observe that the second bracket is at least \( \frac{3}{4} \) if \( r = 3 \) and \( s = 1 \).) \( \Box \)
References


