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On the Inverse Problem for the Graovac–Pisanski Index

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Abstract

The Graovac-Pisanski index is a topological index that at the same time involves graph distances and symmetries of a given graph. In this note it is proved that the values 0, $n/2$, n, $3n/2$, and $2n$ are the only values of the Graovac-Pisanski index (alias modified Wiener index) from the interval $[0, 2n]$ or real numbers that are realizable in the class of all graphs of order n. In the class of trees of order n, only the values 0, n, and $2n$ are realizable.

1 Introduction

The celebrated *Wiener index* [23] of a connected graph G is defined as $W(G) = \sum d_G(u, v)$, where $d_G(u, v)$ is the shortest-path distance in G between the vertices u and v, and the summation runs over all unordered pairs of vertices of G. For its historical developments see the papers collected on the occasion of the 50th anniversary of the index [13] and the survey papers [5, 7, 16]. The wide contemporary interest for the Wiener index can be easily deduced from the recent studies [2, 3, 6, 11, 15, 21] and references therein.

In 1991, Graovac and Pisanski introduced a modified version of the Wiener index with the idea that the new invariant involves, besides the graph distances, also the symmetries of a given graph. In the seminal paper [12] the invariant was names the *modified Wiener index* and renamed in [10] to the *Graovac-Pisanski index* (*GP index* for short). It is defined as follows. If G is a graph, $\mathrm{Aut}(G)$ the automorphism group of G, and $n(G)$ denotes the order of G, then the GP index of G is

$$\widehat{W}(G) = \frac{n(G)}{2|\mathrm{Aut}(G)|} \sum_{x \in V(G)} \sum_{\alpha \in \mathrm{Aut}(G)} d_g(x, \alpha(x)) \,.$$

After its introduction, the GP index received almost no attention, but in the last years the situation is completely different, see [1, 8, 9, 19, 22]. In this note we are interested in the inverse problem for the GP index. In general, the inverse problem asks, for a given (chemical) graph invariant TI and a given value k, find (chemical) graphs G for which $\mathrm{TI}(G) = k$, cf. [14, 18, 20, 24]. In this direction we prove in our main result that the values 0, $n/2$, n, $3n/2$, and $2n$ are the only values of the GP index from the interval $[0, 2n]$ or real numbers that are realizable in the class of all graphs of order n. Moreover, we prove that within the class of trees on n vertices, only the values 0, n, and $2n$ are realizable.

2 Values of the GP index in $[0, 2n]$

Let G be a graph. Recall that the action of $\mathrm{Aut}(G)$ on $V(G)$ partitions $V(G)$ into *orbits.* That is, vertices x and y belong to the same orbit if and only if there exists $\alpha \in \mathrm{Aut}(G)$ such that $\alpha(x) = y$. If $X \subseteq V(G)$, then $W(X)$ is the sum of distances over all unordered pairs of vertices of X. In the seminar paper [12], the following very useful result was proved.

Theorem 2.1 *If G is a connected graph and $V_1, \ldots, V_k$ are the orbits of $V(G)$ under the action of* $\mathrm{Aut}(G)$*, then*

$$\widehat{W}(G) = n(G) \sum_{\mathrm{i}=1}^{\mathrm{k}} \frac{W(V_{\mathrm{i}})}{|V_{\mathrm{i}}|} \,.$$

Before our main result we state a lemma. It is possible that it is already present (in one way or another) in the literature, but we could not find it. To be self-contained, we hence include its proof.

Lemma 2.2 *If G is a connected graph and $X \subseteq V(G)$ is an orbit of cardinality* 3*, then X either induces an independent set or a triangle.*

Proof. Let $X = \{x, y, z\}$. If X induces an independent set there is nothing to prove. Hence suppose that X induces at least one edge, say $xy \in E(G)$. Assume $xz \notin E(G)$. Since x, y, z are in the same orbit, there exists an automorphism $\varphi \in \mathrm{Aut}(G)$ such that $\varphi(x) = z$. Then $\varphi(y) \in \{x, y\}$ and therefore

$$1 = d_G(x, y) = d_G(\varphi(x), \varphi(y)) = d_G(z, \varphi(y))\,.$$

This means that $\varphi(y) = y$ and $yz \in E(G)$. Consider now an automorphism $\alpha \in \mathrm{Aut}(G)$ such that $\alpha(y) = x$. If $\alpha(x) = y$, then $\alpha(z) = z$ and hence

$$2 \le d_G(x, z) = d_G(\alpha(x), \alpha(z)) = d_G(y, z) = 1\,,$$

while if $\alpha(x) = z$, then $\alpha(z) = y$ and hence

$$2 \le d_G(x, z) = d_G(\alpha(x), \alpha(z)) = d_G(z, y) = 1\,.$$

These contradictions prove that $xz \in E(G)$, so X induces a triangle. ■

Let $\mathcal{G}_n$ be the class of simple, connected graphs of order n and let $\widehat{W}[\mathcal{G}_n]$ be the set of all values of the GP index over the graphs from $\mathcal{G}_n$, that is,

$$\widehat{W}[\mathcal{G}_n] = \{\widehat{W}(G) :\ G \in \mathcal{G}_n\}\,.$$

Then our main result reads as follows.

Theorem 2.3 *If $n \ge 6$, then $\widehat{W}[\mathcal{G}_n] \cap [0, 2n] = \{0, n/2, n, 3n/2, 2n\}$.*

Proof. Let $n \ge 6$, let $G \in \mathcal{G}_n$, and assume that $\widehat{W}(G) \le 2n$. Let $V_1, \ldots, V_k$ be the orbits of $V(G)$ under the action of $\mathrm{Aut}(G)$ and let $n_i = |V_i|$, $i \in [k]$. Clearly, if $k = n$ (that is, if $n_i = 1$ for every $i \in [k]$), then $\widehat{W}(G) = 0$. Hence assume in the rest that $k < n$. We may without loss of generality assume that the non-singleton orbits are $V_1, \ldots, V_t$, where $t \le k$. Then

$$\widehat{W}(G) = n \sum_{i=1}^{k} \frac{W(V_i)}{n_i} = n \sum_{i=1}^{t} \frac{W(V_i)}{n_i}\,.$$

For $i \in [t]$ set $\widehat{W_i} = W(V_i)/n_i$, so that $\widehat{W}(G) = n \sum_{i=1}^{t} \widehat{W_i}$. Note that the smallest possible value of $\widehat{W_i}$ is realized if the orbit V_i induces a complete subgraph, in which case we have $\widehat{W_i} = \binom{n_i}{2}/n_i$. Consequently,

$$\widehat{W_i} \in \left\{ \frac{n_i(n_i-1)/2}{n_i}, \frac{(n_i(n_i-1)/2)+1}{n_i}, \ldots \right\},\ i \in [t]\,. \tag{1}$$

If $n_i \geq 5$, then $\widehat{W}_i \geq 2$ by (1), and hence $\widehat{W}(G) \geq 2n$. Hence we may assume in the rest that $n_i \leq 4$ holds for every $i \in [t]$.

Suppose that $V_i = \{x, y\}$. If $d_G(x, y) \geq 5$, then $\widehat{W}_i > 2$ and consequently $\widehat{W}(G) > 2n$. Hence, if $|V_i| = 2$, then $\widehat{W}_i \in \{1/2, 1, 3/2, 2\}$. Consider next an orbit V_i of cardinality 3. From Lemma 2.2 we know that V_i either induces an independent set or a triangle. In the first case $\widehat{W}_i \geq 6/3$ and in the second case $\widehat{W}_i = 1$. We conclude that if $|V_i| = 3$, then $\widehat{W}_i \in \{1, 2\}$. Consider next an orbit of cardinality 4, say $V_i = \{x, y, z, w\}$. From (1) we get that $\widehat{W}_i \in \{6/4, 7/4, 2\}$. We claim that actually $\widehat{W}_i \in \{3/2, 2\}$. Suppose on the contrary that $\widehat{W}_i = 7/4$. Then among the $\binom{4}{2} = 6$ distances between the pairs of vertices of V_i, distance 1 appears five times and distance 2 once, that is, V_i induces the complete graph on four vertices minus an edge. Assume without loss of generality that $xy \notin E(G)$ and consider $\varphi \in \mathrm{Aut}(G)$ such that $\varphi(x) = w$. Then $\varphi(y) \in \{x, y, z\}$ and hence

$$2 = d_G(x, y) = d_G(\varphi(x), \varphi(y)) = d_G(w, \varphi(y)) = 1\,,$$

a contradiction. Thus, if $|V_i| = 4$, then $\widehat{W}_i \in \{3/2, 2\}$.

We have thus proved that if $|V_i| = 2$, then $\widehat{W}_i \in \{1/2, 1, 3/2, 2\}$; if $|V_i| = 3$, then $\widehat{W}_i \in \{1, 2\}$; and if $|V_i| = 4$, then $\widehat{W}_i \in \{3/2, 2\}$. From this it readily follows that $\widehat{W}[\mathcal{G}_n] \cap [0, 2n] \subseteq \{0, n/2, n, 3n/2, 2n\}$.

It remains to show that $\{0, n/2, n, 3n/2, 2n\} \subseteq \widehat{W}[\mathcal{G}_n] \cap [0, 2n]$ holds for every $n \geq 6$. For this sake denote the vertices of the path P_n on n vertices with $v_1, \ldots, v_n$ (with natural edges $v_i v_{i+1}$, $i \in [k-1]$), and for every $n \geq 6$ define the following graphs.

- X_n is the graph obtained from P_{n-1} by adding a new vertex x and the edges xv_1 and xv_2.
- Y_n is the graph obtained from P_{n-1} by adding a new vertex y and the edge yv_2.
- Z_n is the graph obtained from P_{n-2} by adding new vertices z_1 and z_2 and edges v_1z_1, z_1z_2, and z_2v_3.
- W_n is the graph obtained from P_{n-2} by adding new vertices w_1 and w_2 and edges w_1v_2 and w_2v_2.

Clearly, $n(X_n) = n(Y_n) = n(Z_n) = n(W_n) = n$. It is also straightforward to check that $\widehat{W}(X_n) = n/2$, $\widehat{W}(Y_n) = n$, $\widehat{W}(Z_n) = 3n/2$, and $\widehat{W}(W_n) = 2n$. ■

In [17], for a fixed positive integer n, all trees on n vertices are determined that have the maximum value of the GP index. We now complement this classification with the following result which further reduces the variety of the possible values of the GP index for trees. Let $\mathcal{T}_n$ denote the class trees of order n, and let $\widehat{W}[\mathcal{T}_n]$ be the set of all values of the GP index over all trees from $\mathcal{T}_n$. For the proof of our result on trees, the following definitions will be useful. If G is a connected graph, then the *eccentricity* of a vertex $v \in V(G)$ is the maximum distance $d_G(v, x)$ between v and the vertices $x \in V(G)$. The *center* $C(G)$ of G is the set of all vertices of minimum eccentricity.

Theorem 2.4 *If* $n \geq 6$*, then* $\widehat{W}[\mathcal{T}_n] \cap [0, 2n] = \{0, n, 2n\}$*.*

Proof. Let $n \geq 6$ and let $T \in \mathcal{T}_n$. It is well-known that for every tree we have $|C(T)| \in \{1, 2\}$.

Suppose first that $C(T) = \{x\}$. Since automorphisms preserve distances, $C(T)$ forms one of the orbits of $V(T)$ under the action of $\mathrm{Aut}(T)$. If all the other orbits are also singletons, then $\widehat{W}(T) = 0$. Assume next that X is an orbit with $|X| = 2$, say $X = \{u, v\}$. Then, since $d_T(u, v)$ is even, $W(X)/2 \in \mathbb{N}$. Consider next an orbit X of cardinality $|X| = k \geq 3$. Since the vertices from X are pairwise at even distances, we have $W(X)/k \geq 2\binom{k}{2}/2 = k - 1 \geq 2$. It now readily follows that if $\widehat{W}(T) \leq 2n$, then $\widehat{W}(T) \in \{0, n, 2n\}$.

Suppose second that $C(T) = \{x, y\}$. If $C(T)$ forms an orbit of $V(T)$ under the action of $\mathrm{Aut}(T)$, then $W(C(T))/2 = 1/2$. In that case, since $n \geq 6$, an automorphism that transposes the vertices x and y yields an orbit Y containing a neighbor of x (different from y) and a neighbor of y (different from x). For this orbit we then have $W(Y)/|Y| \geq 3/2$ and hence $\widehat{W}(T) \geq 2n$. On the other hand, if x and y are not in the same orbit and T in not asymmetric, then as above we see that for each such orbit Z of cardinality at least 2, we have $W(Z)/|Z| \in \{1, 2\} \cup (2, \infty)$. Hence we can again conclude that if $\widehat{W}(T) \leq 2n$, then $\widehat{W}(T) \in \{0, n, 2n\}$.

To complete the proof note that the families of trees Y_n and Z_n from the proof of Theorem 2.3 yield that $\{0, n, 2n\} \subseteq \widehat{W}[\mathcal{T}_n] \cap [0, 2n]$ holds for every $n \geq 6$. ■

We note that if n is odd, then Theorem 2.3 can be deduced by combining Theorem 2.3 with the main result of [4].

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