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ON THE GRAOVAC-PISANSKI INDEX OF A GRAPH

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Abstract. Let G be a graph. Its Graovac-Pisanski index is

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

where $\mathrm{Aut}(G)$ is the group of automorphisms of G, and its Wiener index, $W(G)$, is the sum of all distances in G. In the class of trees (unicyclic graphs) on n vertices we find those with the maximum value of Graovac-Pisanski index. We show that the inequality $\mathrm{GP}(G) \leq W(G)$ is not true in general, but it is true for trees.

1. Introduction

In 1947 Wiener introduced the famous Wiener index [**5**], defined as the sum of distances between all pairs of vertices of a graph. Since then, many molecular descriptors have appeared. One of them is the Graovac-Pisanski index [**3**], which is also based on distances but its advantage is in considering also the symmetries of a graph. Similarly as Wiener showed a correlation of the Wiener index of alkanes with their boiling points [**5**], Črepnjak et al. showed that the Graovac-Pisanski index of some hydrocarbon molecules is correlated with their melting points [**1**].

Let G be a graph. By $V(G)$ and $E(G)$ we denote its vertex and edge sets, respectively. For two vertices u and v, by $\mathrm{dist}(u, v)$ we denote the distance from u to v. The Wiener index of a graph, $W(G)$, is the sum of all distances in a graph, i.e.,

$$W(G) = \sum_{u,v \in V(G)} \mathrm{dist}(u, v).$$

On the other hand, the Graovac-Pisanski index of G, $\mathrm{GP}(G)$, (originally called a modified Wiener index) is defined as

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

where $\mathrm{Aut}(G)$ is the group of automorphisms of G. The group of automorphisms of G partitions $V(G)$ into orbits. We say that $u, v \in V(G)$ belong to the same orbit

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if there is an automorphism $\alpha \in \mathrm{Aut}(G)$ such that $\alpha(u) = v$. Let $V_1, V_2, \dots, V_t$ be all the orbits of $\mathrm{Aut}(G)$ in G. In [**3**] it was shown that for every graph G

$$\mathrm{GP}(G) = |V(G)| \cdot \sum_{i=1}^{t} \frac{W_G(V_i)}{|V_i|}, \tag{1}$$

where $V_1, V_2, \dots, V_t$ are the orbits of $\mathrm{Aut}(G)$ and $W_G(V_i) = \sum_{u,v \in V_i} \mathrm{dist}(u, v)$. For $U \subseteq V(G)$ and $v \in V(G)$, we denote $w_U(v) = \sum_{u \in U} \mathrm{dist}(u, v)$. Since all vertices u in an orbit U have the same value of $w_U(u)$, we can rewrite (1) in the following way

$$\mathrm{GP}(G) = |V(G)| \cdot \sum_{i=1}^{t} \tfrac{1}{2} \cdot w_{V_i}(v_i), \tag{2}$$

where $V_1, V_2, \dots, V_t$ are the orbits of $\mathrm{Aut}(G)$ and $v_1, v_2, \dots, v_t$, respectively, are their representatives. Using (2) one can see that the Graovac-Pisanski index of every graph is either an integer or half of an integer. Moreover, in [**2**] it was shown that the Graovac-Pisanski index of a bipartite graph is an integer.

In this paper (talk) we survey our current results on Graovac-Pisanski index, which are at the time of submission of this note still unpublished.

2. Comparison with Wiener index

As mentioned already in [**3**], $\mathrm{GP}(G) = W(G)$ if G is vertex-transitive, i.e., if there is just one orbit of vertices of $\mathrm{Aut}(G)$ (see (1)). On the other hand, if G has $|V(G)|$ orbits of $\mathrm{Aut}(G)$ then $\mathrm{GP}(G) = 0$. Regarding the number of orbits these two cases are extremal, and so one can expect that $0 \le \mathrm{GP}(G) \le W(G)$. While the inequality $0 \le \mathrm{GP}(G)$ follows from the definition and it is obvious that $\mathrm{GP}(G) = 0$ if and only if G has $|V(G)|$ orbits, the inequality $\mathrm{GP}(G) \le W(G)$ is not so obvious although one can object that all the distaces contribute to $W(G)$ while only some of them contribute to $\mathrm{GP}(G)$. The problem is caused by the normalizing factors $|V(G)|$ and $\frac{1}{|V_i|}$ in (1). From the terms in (1) one can deduce that $W(G) - \mathrm{GP}(G)$ can be negative if there are "big distances" inside orbits and "small distances" between them. A typical example of such a situation is the complete bipartite graph $K_{a,b}$, where $a \neq b$. We have the following statement.

Proposition 1. *If $a > b \ge 2$ then*

$$W(K_{a,b}) - \mathrm{GP}(K_{a,b}) = a + b - ab < 0,$$

that is $W(K_{a,b}) < \mathrm{GP}(K_{a,b})$.

There is no complete bipartite graph $K_{a,b}$ with $a > b$ for which $W(K_{a,b}) = \mathrm{GP}(K_{a,b})$. But there are graphs G which are not vertex-transitive and though $W(G) = \mathrm{GP}(G)$.

Now we turn our attention to trees. By P_n we denote a path on n vertices. Since every tree has at most two central vertices and since vertices which are central cannot be in the same orbit as non-central ones, P_1 and P_2 are the only trees which have just one orbit of the group of automorphisms, i.e., which are vertex-transitive. Hence, $W(T) = \mathrm{GP}(T)$ if T is P_1 or P_2. For all other trees, considering the contribution of every edge to $W(G)$ and $\mathrm{GP}(G)$, we prove the following statement.

Theorem 2. *Let T be a tree on at least three vertices. Then*

$$W(T) > \mathrm{GP}(T).$$

Since trees are bipartite graphs, $\mathrm{GP}(T)$ is a nonnegative integer if T is a tree. We prove the following theorem.

Theorem 3. *There exists a tree T satisfying $W(T) - \mathrm{GP}(T) = \ell$ if and only if ℓ is integer, $\ell \geq 0$ and $\ell \notin \{3, 4\}$.*

3. Extremal graphs

As mentioned above, $\mathrm{GP}(G) = 0$ if and only if $\mathrm{Aut}(G)$ has just the trivial automorphism. This answers the question of finding graphs with the minimum value of Graovac-Pisanski index. As regards the other extremum, we have the following result.

Theorem 4. *Let T be a tree on n vertices with the maximum value of Graovac-Pisanski index. Then T is either the path P_n, or H_n, or $K_{1,3}$, or $K_{1,4}$ or T_7. Moreover,*

$$\mathrm{GP}(T) = \begin{cases} \dfrac{n^3 - n}{8} & \text{if } n \text{ is odd,} \\ \dfrac{n^3}{8} & \text{if } n \text{ is even.} \end{cases}$$

Here, H_n is obtained from P_{n-4} with endvertices v_1 and v_2 when two pendant vertices are attached to v_1 and two pendant vertices are attached to v_2. The graph T_7 is obtained from $K_{1,3}$ by subdividing each edge exactly once. By Theorem 4, if $n \geq 8$ then there are exactly two trees with the maximum value of Graovac-Pisanski index.

As regards unicyclic graphs, we have the following statement.

Theorem 5. *Let G be a unicyclic graph on n vertices with the maximum value of Graovac-Pisanski index. Then G is the n-cycle and*

$$\mathrm{GP}(G) = \begin{cases} \dfrac{n^3 - n}{8} & \text{if } n \text{ is odd,} \\ \dfrac{n^3}{8} & \text{if } n \text{ is even.} \end{cases}$$

Observe that the maximum value of Graovac-Pisanski index in the class of trees is the same as in the class of unicyclic graphs. We conjecture that we obtain the same value if one extends trees (unicyclic graphs) to the class of all graphs on n vertices.

Theorems 4 and 5 were obtained using the fact that every automorphism of a tree (a cycle) fixes the center (the cycle). Then we generalized the Graovac-Pisanski index. Finally, in a sequence of steps we modified the graph so that in every step we increased the generalized Graovac-Pisanski index and we terminated in an extremal graph.

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