Graovac-Pisanski index for trees

Martin Knor

(joint work with Riste Škrekovski and Aleksandra Tepeh)

Graovac-Pisanski index, originally called a modified Wiener index, was introduced in 1991. Let G be a graph. Its Graovac-Pisanski 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 and $\mathrm{dist}(u, v)$ is the distance from u to v in G. Recall that Wiener index of G is

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

While Wiener index is correlated with the boiling points of alcanes, Graovac-Pisanski index is correlated with the melting points of some types of hydrocarbon molecules. For $U \subseteq V(G)$ and $v \in V(G)$ we define $w_U(v) = \sum_{u \in U} \mathrm{dist}(u, v)$. It is easy to see that

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

where $V_1, V_2, \ldots, V_t$ are the orbits of $\mathrm{Aut}(G)$ in G and $v_1, v_2, \ldots, v_t$ are their representatives, respectively. Consequently, $\mathrm{GP}(G)$ is an integer number if G is a tree (in fact, $\mathrm{GP}(G)$ is integer if G is a bipartite graph). We prove that $0 \le \mathrm{GP}(T) \le W(T)$ if T is a tree. While the first inequality is trivially true for all graphs, we show that the second does not hold in general. Also, we determine all values ℓ for which there is a tree T such that $W(T) - \mathrm{GP}(T) = \ell$. Further, in the class of trees on n vertices we find those with the maximum value of Graovac-Pisanski index.

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