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Comparing Zagreb M_1 and M_2 indices for acyclic molecules

Damir Vukičević*

Department of Mathematics, University of Split, Nikole Tesle 12, HR-21000 Split, Croatia

E-mail: vukicevi@pmfst.hr

Ante Graovac

Faculty of Science, University of Split, Nikole Tesle 12, HR-21000 Split, Croatia and The R. Bošković Institute, P.O.B. 180, HR-10002 Zagreb, Croatia

E-mail: graovac@irb.hr

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Abstract

Recently, it has been conjectured that for each simple graph $G=(V,E)$ with $n=|V|$ vertices and $m=|E|$ edges, it holds $M_1/n \le M_2/m$, where M_1 and M_2 are the first and second Zagreb index. This claim has been disproved in [1] for connected as well as for disconnected graphs. Here, we show that this claim holds for trees.

Introduction

The first and second Zagreb indices are among the oldest and the most famous topological indices (see [2-5] and references within) and they are defined as:

$$M_1 = \sum_{i \in V} d_i^2 \text{ and } M_2 = \sum_{(i,j) \in E} d_i d_j ,$$

* The author to whom correspondece should be addressed

where V is the set of vertices, E is set of edges and d_i is degree of vertex i. Recently, the system AutoGraphiX [6-7] proposed the following conjecture:

Conjecture 1. For all simple connected graphs G,

$$M_1 / n \le M_2 / m$$

and the bound is tight for complete graphs.□

However, in paper [1], it has been proved that in general this conjecture is not true. But, it has been proved that this conjecture is true if we restrict our analysis to the graphs with maximal degree at most four. This result has been of interest since the Zagreb index is widely used [2,3] in the study of hydrocarbons whose maximal degree is indeed at most 4. Also, the Zagreb index is often used in study of acyclic compounds (alkanes and molecules similar to them [2,3]), hence it is of interest to check if the Conjecture 1 holds for acyclic molecules. In this paper as a sequel of the study of this conjecture [1,8], we show that the conjecture holds for acyclic molecules with no restrictions on the degree of vertices. Moreover the equality holds only for star-like molecules.

Main results

Theorem 1. Let v be vertex of tree T such that $d_v \ge 2$. Then, $M_1 - M_2 \le d_v$.

Proof: Denote by $u_1,...,u_{d_v}$ neighbors of v. Denote by T_i component of graph $T-v$ that contains u_i. Denote $E_i = E(T_i) \cup \{vu_i\}$. Note that $E(T)$ can be decomposed as $E(T) = E_1 \cup E_2 \cup ... \cup E_{d_v}$. Hence,

$$M_1 - M_2 = \sum_{i\in V} d_i^2 - \sum_{ij\in E} d_i \cdot d_j = \sum_{i\in V}\sum_{\substack{j\in V\\ ij\in E}} d_i - \sum_{ij\in E} d_i \cdot d_j = \sum_{ij\in E}\left(d_i + d_j\right) - \sum_{ij\in E} d_i \cdot d_j$$

$$= \sum_{ij\in E}\left(d_i + d_j - d_i d_j\right) = \sum_{q=1}^{d_v}\sum_{ij\in E_q}\left(d_i + d_j - d_i d_j\right).$$

Therefore, it is sufficient to prove that $\alpha(T_q) \equiv \sum_{ij\in E_q}\left(d_i + d_j - d_i d_j\right) \le 1$ for each $q = 1,...,d_v$. We prove the claim by induction on the number of vertices in T_q.

If $T_q = 1$, then $E_q = \{uv_q\}$ and $d_{v_q} = 1$. Hence, $\sum_{ij\in E_q}\left(d_i + d_j - d_i d_j\right) = d_v + 1 - 1\cdot d_v = 1$ and the claim is proved. Now, suppose that T_q has x vertices and that claim holds for all graphs with less then x vertices. Suppose to the contrary that $\alpha(T_q) = \sum_{ij\in E_q}\left(d_i + d_j - d_i d_j\right) > 1$. Let l be any leaf, namely any vertex of degree 1, in T_q (different from u_q). Denote by m the only neighbor of l, by $N(m)$ set of neighbors of m, and by E_m the set of all edges incident to m. Note that $N(m)$ contains l and at least one more vertex. From the induction hypothesis, it follows that $\alpha(T_q - l) < \alpha(T_q)$, hence:

$$
\begin{aligned}
&0 < \alpha(T_q) - \alpha(T_q - l) = \\
&= \sum_{ij \in E_q} (d_i + d_j - d_i d_j) - \left[\sum_{ij \in E_q \setminus M} (d_i + d_j - d_i d_j) + \sum_{\substack{im \\ i \in N(m) \setminus \{l\}}} \left(d_i + (d_m - 1) - d_i \cdot (d_m - 1)\right) \right] \\
&= (d_l + d_m - d_l \cdot d_m) - \sum_{\substack{im \\ i \in N(m) \setminus \{l\}}} \left([d_i + d_m - d_i d_m] - [d_i + (d_m - 1) - d_i \cdot (d_m - 1)] \right) \\
&= 1 - \sum_{\substack{im \\ i \in M \setminus \{l\}}} (1 + d_i),
\end{aligned}
$$

which is a contradiction. This proves the theorem. ■

From here, it can be proved that:

Theorem 2. Let T be a tree with at least two vertices. Then, $\frac{M_1}{n} \leq \frac{M_2}{m}$. The equality holds if and only if T is star.

Proof: If $T = K_2$, the claim obviously holds, hence suppose that $T \neq K_2$. Let v be vertex of the smallest degree d_v larger then 1. Since no two vertices of degree 1 are adjacent, it follows that $M_2 \geq m \cdot d_v$. We have:

$$
\begin{aligned}
&\frac{M_1}{M_2} \leq \{\text{from Theorem 1}\} \leq \frac{M_2 + d_v}{M_2} = 1 + \frac{d_v}{M_2} \leq \left\{ \begin{array}{l} \text{the last expression is decreasing in } M_2, \\ \text{hence, it is minimal for } M_2 = m \cdot d_v \end{array} \right\} \leq \\
&\overset{(*)}{\leq} 1 + \frac{d_v}{m \cdot d_v} = \frac{m+1}{m} = \{T \text{ is tree, hence } m = n - 1\} = \frac{n}{m}.
\end{aligned}
$$

From here, it follows that: $\frac{M_1}{n} \leq \frac{M_2}{m}$. Moreover if $(*)$ is equality, then T is connected bipartite graph whose one class consists of vertices of degree 1. Hence, T is a star. On the other hand, for all stars $\frac{M_1}{n} \leq \frac{M_2}{m}$. ■

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