MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **60** (2008) 37-44

ISSN 0340 - 6253

Comparing variable Zagreb M_1 and M_2 indices for acyclic molecules

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(Received April 4, 2007)

Abstract

Recently, it has been conjectured that $M_1/n \le M_2/m$ holds for each simple graph $G=(V,E)$ with $n=|V|$ vertices and $m=|E|$ edges, 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, but it was shown that it holds for trees [2]. Here, we analyze generalizations of this claim for variable Zagreb indices of trees.

Introduction

The first and second Zagreb indices are among the oldest and best known topological indices (see [3-6] and references within) and they are defined as:

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

where V is the set of vertices, E is set of edges and d_i is degree of vertex i. These indices have been generalized to variable first and second Zagreb indices [7] defined as

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

Recently, the system AutoGraphiX [8-9] proposed the following conjecture:

Conjecture 1. For all simple connected graphs G,

$$M_1 / n \leq M_2 / m$$

and the bound is tight for complete graphs.□

In paper [1], this claim has been disproved for general graphs and in paper [2] it has been proved for trees. In paper [10] the generalization of this claim to the variable Zagreb indices have been analyzed for general graphs. Here, in the fourth paper in this series, we analyze variable Zagreb indices for trees.

We prove as our main result that:

Theorem 2. ${}^{\lambda}M_1 / n \leq {}^{\lambda}M_2 / m$ for all trees if and only if $\lambda \in \left[0,1\right]$.

Main results

The following Theorems A and B are given in paper [10] and Theorem C is given in paper [2]:

Theorem A. For all graphs G and all $\lambda \in \left[0,1/2\right]$, it holds that ${}^{\lambda}M_1\left(G\right)/n \leq {}^{\lambda}M_2\left(G\right)/m$.

Theorem B. Let $\lambda \in R \backslash \left[0,1\right]$ and G be any complete unbalanced bipartite graph. Then, ${}^{\lambda}M_1\left(G\right)/n > {}^{\lambda}M_2\left(G\right)/m$.

Here, unbalanced refers to different cardinalities of *white* and *black* vertices and complete denotes the fact that each *white* vertex is adjacent to all *black* vertices.

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

Since a star with at least three vertices is an unbalanced complete bipartite graph, it follows that it is sufficient to prove:

Proposition 3. ${}^{\lambda}M_1/n \leq {}^{\lambda}M_2/m$ for all trees and for all $\lambda \in (1/2,1)$.

First, we prove that:

Proposition 4. Let v be vertex of tree T such that $d_v \geq 2$. Then, ${}^{\lambda}M_1 - {}^{\lambda}M_2 \leq d_v^{\lambda}$ for all $\lambda \in (1/2,1)$.

Proof: Using the notation given in [2], we denote by $u_1,...,u_{d_v}$ the neighbors of v, by T_i the component of graph $T-v$ that contains u_i, by $E_i = E(T_i) \cup \{vu_i\}$. Set $E(T)$ is decomposed as $E(T) = E_1 \cup E_2 \cup ... \cup E_{d_v}$. Similarly, as in [2], it can be shown that

$$ {}^{\lambda}M_1 - {}^{\lambda}M_2 = \sum_{q=1}^{d_v} \sum_{ij \in E_q} \left(d_i^{2\lambda-1} + d_j^{2\lambda-1} - d_i^{\lambda} d_j^{\lambda} \right). $$

Therefore, it is sufficient to prove that $\alpha(T_q) \equiv \sum_{ij \in E_q} \left(d_i^{2\lambda-1} + d_j^{2\lambda-1} - d_i^{\lambda} d_j^{\lambda} \right) \leq d_v^{\lambda-1}$ 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, $\sum_{ij \in E_q} \left(d_i^{2\lambda-1} + d_j^{2\lambda-1} - d_i^{\lambda} d_j^{\lambda} \right) = d_v^{2\lambda-1} + 1 - d_v^{\lambda}$. We need to prove that: $d_v^{2\lambda-1} + 1 - d_v^{\lambda} \leq d_v^{\lambda-1}$, i.e. that:

$$ d_v^{2\lambda-1} + d_v^{0} \leq d_v^{\lambda-1} + d_v^{\lambda}. $$

This follows from the fact that $f_1(t) = d_v^t$ is a convex function ($f_1''(t) = d_v^t \cdot (\ln d_v)^2$). 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 $\alpha(T_q) \equiv \sum_{ij \in E_q} \left(d_i^{2\lambda-1} + d_j^{2\lambda-1} - d_i^{\lambda} d_j^{\lambda} \right) > d_v^{\lambda-1}$. Proceeding analogously as in [2], let l be any leaf, namely any vertex of degree 1, in T_q (different from u_q). Denote by l' the only neighbor of l and by $N(l')$ the set of neighbors of l'. Note that $N(l')$ contains at least one vertex which is not a leaf. From the induction hypothesis, it follows that $\alpha(T_q - l) < \alpha(T_q)$, hence:

$$ \begin{aligned} & 0 < \alpha(T_q) - \alpha(T_q - l) = \\ & = \sum_{ij \in E_q} \left(d_i^{2\lambda-1} + d_j^{2\lambda-1} - d_i^{\lambda} d_j^{\lambda} \right) - \\ & - \left[\sum_{ij \in E_q \setminus M} \left(d_i^{2\lambda-1} + d_j^{2\lambda-1} - d_i^{\lambda} d_j^{\lambda} \right) + \sum_{\substack{im \in E_q \\ i \in N(m) \setminus \{l\}}} \left(d_i^{2\lambda-1} + (d_{l'} - 1)^{2\lambda-1} - d_i^{\lambda} \cdot (d_{l'} - 1)^{\lambda} \right) \right] \end{aligned} $$

$$=\left(d_l^{2\lambda-1}+d_{l'}^{2\lambda-1}-d_l^{\lambda}\cdot d_{l'}^{\lambda}\right)-$$
$$\sum_{\substack{il'\in E_q\\ i\in N(l')\setminus\{l\}}}\left(\left[d_i^{2\lambda-1}+d_{l'}^{2\lambda-1}-d_i^{\lambda}d_{l'}^{\lambda}\right]-\left[d_i^{2\lambda-1}+\left(d_{l'}-1\right)^{2\lambda-1}-d_i^{\lambda}\cdot\left(d_{l'}-1\right)^{\lambda}\right]\right)$$
$$=\left(1+d_{l'}^{2\lambda-1}-d_{l'}^{\lambda}\right)+\sum_{\substack{il'\in E_q\\ i\in N(l')\setminus\{l\}}}\left(\left[d_{l'}^{2\lambda-1}-d_i^{\lambda}d_{l'}^{\lambda}\right]-\left[\left(d_{l'}-1\right)^{2\lambda-1}-d_i^{\lambda}\cdot\left(d_{l'}-1\right)^{\lambda}\right]\right).$$

In order to obtain a contradiction, it is sufficient to prove the following two claims

Claim A $\left[d_{l'}^{2\lambda-1}-d^{\lambda}d_{l'}^{\lambda}\right]-\left[\left(d_{l'}-1\right)^{2\lambda-1}-d^{\lambda}\cdot\left(d_{l'}-1\right)^{\lambda}\right]\le 0$ for each $d\in N$.

Claim B $\left(1+d_{l'}^{2\lambda-1}-d_{l'}^{\lambda}\right)+\left(\left[d_{l'}^{2\lambda-1}-d^{\lambda}d_{l'}^{\lambda}\right]-\left[\left(d_{l'}-1\right)^{2\lambda-1}-d^{\lambda}\cdot\left(d_{l'}-1\right)^{\lambda}\right]\right)\le 0$ for each $d\in N$, $d\ge 2$.

Let us prove Claim A:

Proof of Claim A: Note that left hand-side is decreasing in d, hence it is sufficient to prove it for $d=1$, i.e. we need to prove that:

$$\left[d_{l'}^{2\lambda-1}-\left(d_{l'}-1\right)^{2\lambda-1}\right]-\left[d_{l'}^{\lambda}-\left(d_{l'}-1\right)^{\lambda}\right]\le 0.$$

Since $2\lambda-1<\lambda$, it is sufficient to prove that function $f_2(t)=d_{l'}^{t}-\left(d_{l'}-1\right)^{t}$ is increasing function on $(1/2,1)$ and this follows form $f_2'(t)=d_{l'}^{t}\cdot\ln\left(d_{l'}\right)-\left(d_{l'}-1\right)^{t}\cdot\ln\left(d_{l'}-1\right)>0$.■

Now, let us prove Claim B:

Proof of Claim B: Again, note that left hand-side is decreasing in d, hence it is sufficient to prove it for $d=2$, i.e. we need to prove that:

$$\left(1+d_{l'}^{2\lambda-1}-d_{l'}^{\lambda}\right)+\left(\left[d_{l'}^{2\lambda-1}-2^{\lambda}d_{l'}^{\lambda}\right]-\left[\left(d_{l'}-1\right)^{2\lambda-1}-2^{\lambda}\cdot\left(d_{l'}-1\right)^{\lambda}\right]\right)\le 0.$$

This expression can be rewritten as:

$$\left(1+d_{l'}^{2\lambda-1}-d_{l'}^{\lambda}\right)+\left(1-2^{\lambda}\right)\cdot\left(d_{l'}^{\lambda}-\left(d_{l'}-1\right)^{\lambda}\right)+\left(\left[d_{l'}^{2\lambda-1}-d_{l'}^{\lambda}\right]-\left[\left(d_{l'}-1\right)^{2\lambda-1}-\left(d_{l'}-1\right)^{\lambda}\right]\right)\le 0. \quad (*)$$

Let us distinguish four cases:

CASE 1: $d_{l'}=2$.

In this case (*) becomes $\left(1+2^{2\lambda-1}-2^{\lambda}\right)+\left(1-2^{\lambda}\right)\cdot\left(2^{\lambda}-1\right)+\left(\left[2^{2\lambda-1}-2^{\lambda}\right]\right)\le 0$ and here equality obviously holds.

CASE 2: $\lambda \le 0.99$, $d_{l'} \ge 35$.

From the proof of Claim A, it follows that the third summand in (*) is negative, the second summand is obviously negative, hence (*) holds if $1+d_{l'}^{2\lambda-1}-d_{l'}^{\lambda} \le 0$. Note that $f_3(t)=1+t^{2\lambda-1}-t^{\lambda}$ is decreasing on $(1,+\infty)$ in d, because $2\lambda-1<\lambda$ implies that $f_3'(t)=(2\lambda-1)\cdot t^{2\lambda-2}-\lambda\cdot t^{\lambda-1}=t^{-1}\left[(2\lambda-1)\cdot t^{2\lambda-1}-\lambda\cdot t^{\lambda}\right]<0$. Hence, it is sufficient to show that $1+35^{2\lambda-1}-35^{\lambda} \le 0$. The last inequality can be rewritten as $\frac{1}{35}\cdot\left(35^{\lambda}\right)^2-35^{\lambda}+1\le 0$. Solving $\frac{1}{35}\cdot t^2-t+1\le 0$ one gets: $\frac{1}{2}\left(35-\sqrt{1085}\right)\le t\le\frac{1}{2}\left(35+\sqrt{1085}\right)$. Note that $\frac{1}{2}\left(35-\sqrt{1085}\right)\le 35^{1/2}\le 35^{\lambda}\le 35^{0.99}\le\frac{1}{2}\left(35+\sqrt{1085}\right)$, hence this case is proved.

CASE 3: $\lambda \le 0.99$, $3 \le d_{l'} < 34$.

Let $f_d, f_u : (0.5, 0.99) \to \{0.500, 0.501, ..., 0.989, 0.990\}$ be two functions that round down and up the number to the nearest $1/1000$. More formally $f_d(t)=\frac{1}{1000}\cdot\lceil 1000t\rceil$ and $f_u(t)=\frac{1}{1000}\cdot\lceil 1000t\rceil$, where $\lfloor t\rfloor$ is the greatest integer $\le t$ and $\lceil t\rceil$ is the smallest integer $\ge t$. Note that:

$$\left(1+d_{l'}^{2\lambda-1}-d_{l'}^{\lambda}\right)+\left(1-2^{\lambda}\right)\cdot\left(d_{l'}^{\lambda}-\left(d_{l'}-1\right)^{\lambda}\right)+\left(\left[d_{l'}^{2\lambda-1}-d_{l'}^{\lambda}\right]-\left[\left(d_{l'}-1\right)^{2\lambda-1}-\left(d_{l'}-1\right)^{\lambda}\right]\right)\le$$
$$\le\left(1+d_{l'}^{2f_u(\lambda)-1}-d_{l'}^{f_d(\lambda)}\right)+\left(1-2^{f_d(\lambda)}\right)\cdot\left(d_{l'}^{f_d(\lambda)}-\left(d_{l'}-1\right)^{f_u(\lambda)}\right)+$$
$$\left(\left[d_{l'}^{2f_u(\lambda)-1}-d_{l'}^{f_d(\lambda)}\right]-\left[\left(d_{l'}-1\right)^{2f_d(\lambda)-1}-\left(d_{l'}-1\right)^{f_u(\lambda)}\right]\right).$$

Hence, it is sufficient to prove that:

$$\left(1+d^{2(t+0.001)-1}-d^{t}\right)+\left(1-2^{t}\right)\cdot\left(d^{t}-(d-1)^{(t+0.001)}\right)+$$
$$\left(\left[d^{2(t+0.001)-1}-d^{t}\right]-\left[(d-1)^{2t-1}-(d-1)^{(t+0.001)}\right]\right)\le 0.$$

For each $3\le d\le 34$ and each $t\in\{0.500, 0.501, ..., 0.989\}$ a computer check shows that this is true.

CASE 4: $\lambda > 0.99, d \ge 3$.

From the proof of Claim 1, it follows that it is sufficient to prove that:

$$\left(1+d_{l'}^{2\lambda-1}-d_{l'}^{\lambda}\right)+\left(1-2^{\lambda}\right)\cdot\left(d_{l'}^{\lambda}-\left(d_{l'}-1\right)^{\lambda}\right)\leq 0,$$

or equivalently that:

$$d_{l'}^{\lambda}-d_{l'}^{2\lambda-1}+\left(2^{\lambda}-1\right)\cdot\left(d_{l'}^{\lambda}-\left(d_{l'}-1\right)^{\lambda}\right)-1\geq 0.$$

Using the Lagrange theorem, one gets that $d_{l'}^{\lambda}-d_{l'}^{2\lambda-1}=\ln d_{l}\cdot\left(1-\lambda\right)\cdot d_{l'}^{t}$ for some $t\in\left(2\lambda-1,\lambda\right)$. Hence,

$$d_{l'}^{\lambda}-d_{l'}^{2\lambda-1}\geq \ln d_{l'}\cdot\left(1-\lambda\right)\cdot d_{l'}^{2\lambda-1}.$$

Analogously, $d_{l'}^{\lambda}-\left(d_{l'}-1\right)^{\lambda}=1\cdot\lambda\cdot t^{\lambda-1}$ for some $t\in\left(d_{l'}-1,d_{l'}\right)$. Hence,

$$d_{l'}^{\lambda}-\left(d_{l'}-1\right)^{\lambda}\geq 1\cdot\lambda\cdot d_{l'}^{\lambda-1}.$$

It follows that:

$$\begin{aligned}&d_{l'}^{\lambda}-d_{l'}^{2\lambda-1}+\left(2^{\lambda}-1\right)\cdot\left(d_{l'}^{\lambda}-\left(d_{l'}-1\right)^{\lambda}\right)-1\geq \ln d_{l'}\cdot\left(1-\lambda\right)\cdot d_{l'}^{2\lambda-1}+\lambda\cdot d_{l'}^{\lambda-1}-1\geq\\&\geq\left(1-\lambda\right)\cdot d_{l'}^{2\lambda-1}+\lambda\cdot d_{l'}^{\lambda-1}-1.\end{aligned}$$

Therefore, it is sufficient to prove that:

$$\left(1-\lambda\right)\cdot d_{l'}^{2\lambda-1}+\lambda\cdot d_{l'}^{\lambda-1}-1\geq 0.$$

Note that function $f_4\left(t\right)=\left(1-\lambda\right)t^{2\lambda-1}+\lambda\cdot t^{\lambda-1}$ is strictly increasing on $\left[3,+\infty\right)$, because

$$f_4'(t)=\left(1-\lambda\right)\left(2\lambda-1\right)t^{2\lambda-1}+\lambda\cdot\left(\lambda-1\right)t^{\lambda-1}=\left(1-\lambda\right)\cdot t^{\lambda-1}\cdot\left(\left(2\lambda-1\right)\cdot t-\lambda\right)>0.$$

Hence, it is sufficient to prove that:

$$\left(1-\lambda\right)\cdot 3^{2\lambda-1}+\lambda\cdot 3^{\lambda-1}-1\geq 0.$$

Substituting $t=3^{\lambda}$, the last inequality is transformed to:

$$\frac{1-\lambda}{3}\cdot t^2+\frac{\lambda}{3}\cdot t-1\geq 0.$$

By taking into the account that $(1-\lambda)/3>0$ one gets that it is sufficient to show that:

$$t\geq\frac{\lambda}{2\left(-1+\lambda\right)}+\frac{1}{2}\sqrt{\frac{12-12\lambda+\lambda^2}{\left(-1+\lambda\right)^2}},$$

i.e. that:

$$3^{\lambda} \geq \frac{\sqrt{\lambda^2 - 12\lambda + 12} - \lambda}{2(1-\lambda)}.$$

The last inequality can be rewritten as:

$$3^{\lambda} \geq \frac{12 - 12\lambda}{2(1-\lambda)\cdot\left(\sqrt{\lambda^2 - 12\lambda + 12} + \lambda\right)}$$

$$3^{\lambda} \geq \frac{6}{\sqrt{\lambda^2 - 12\lambda + 12} + \lambda}$$

Since, $\sqrt{\lambda^2 - 12\lambda + 12} + \lambda \geq 2\sqrt[4]{\left(\lambda^2 - 12\lambda + 12\right)\cdot\lambda^2}$, it is sufficient to prove that:

$$3^{\lambda} \geq \frac{3}{\sqrt[4]{\left(\lambda^2 - 12\lambda + 12\right)\cdot\lambda^2}}$$

$$\ln\left(\lambda^4 - 12\lambda^3 + 12\cdot\lambda^2\right) \geq (4 - 4\lambda)\cdot\ln 3.$$

Since, left and right-hand sides are equal to 0 for $\lambda = 1$, it is sufficient to prove that the first derivative of the left hand-side is smaller then the first derivative of the right hand-side, i.e. that:

$$\frac{4\lambda^3 - 36\lambda^2 + 24\lambda}{\lambda^4 - 12\lambda^3 + 12\cdot\lambda^2} \leq -4\ln 3,$$

or equivalently that:

$$\frac{-4\lambda^3 + 36\lambda^2 - 24\lambda}{\lambda^4 - 12\lambda^3 + 12\cdot\lambda^2} \geq 4\ln 3.$$

This follows from:

$$\frac{-4\lambda^3 + 36\lambda^2 - 24\lambda}{\lambda^4 - 12\lambda^3 + 12\cdot\lambda^2} \geq \frac{-4\cdot 1^3 + 36\cdot 0.99^2 - 24\cdot 1}{1^4 - 12\cdot 0.99^3 + 12\cdot 1^2} = \frac{7.2836}{1.356412} \geq 5 \geq 4\ln 3.$$

This proves Claim B. ■

From Proposition 4, the proof of Proposition 3 goes in a complete analogy with the proof of Theorem 2 in [2]:

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 ${}^{\lambda}M_2 \geq m \cdot (1 \cdot d_v)^{\lambda}$. We have:

$$\frac{{}^{\lambda}M_1}{{}^{\lambda}M_2} \leq \{\text{from Theorem 1}\} \leq \frac{{}^{\lambda}M_2 + d_v{}^{\lambda}}{{}^{\lambda}M_2} = 1 + \frac{d_v{}^{\lambda}}{{}^{\lambda}M_2} \leq \left\{\begin{array}{l}\text{the last expression is decreasing in } {}^{\lambda}M_2, \\ \text{hence, it is minimal for } {}^{\lambda}M_2 = m \cdot d_v\end{array}\right\} \leq$$

$$\leq 1 + \frac{d_v{}^{\lambda}}{m \cdot d_v{}^{\lambda}} = \frac{m+1}{m} = \{T \text{ is tree, hence } m = n-1\} = \frac{n}{m}.$$

From here, it follows that: ${}^{\lambda}M_1 / n \leq {}^{\lambda}M_2 / m$. ■

Acknowledgment

Partial support of the Croatian Ministry of Science, Education and Sports (Grants "Mathematical models in chemistry" and "Modeling of molecules and materials by methods of mathematical and computational chemistry") is gratefully acknowledged.

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