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Comparing variable Zagreb indices for unicyclic graphs

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Abstract

Variable first and second Zagreb indices are defined by ${}^{\lambda}M_1(G) = \sum_{v_i \in V} d_i^{2\lambda}$ and ${}^{\lambda}M_2(G) = \sum_{v_iv_j \in E} d_i^{\lambda} \cdot d_j^{\lambda}$, where d_i is the degree of the vertex v_i and λ is any real number. In this note, we obtain ${}^{\lambda}M_2(G) \geq {}^{\lambda}M_1(G)$ for all unicyclic graphs and all $\lambda \in [0, 1]$.

1 Introduction.

For a molecular graph $G = (V, E)$, the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ are defined in [1-3] as

$$M_1(G) = \sum_{v_i \in V} d_i^2 \quad \text{and} \quad M_2(G) = \sum_{v_iv_j \in E} d_i \cdot d_j \,,$$

where d_i denotes the degree of the vertex v_i of G. Recently, it has been conjectured that for each simple graph $G = (V, E)$ with $n = |V|$ vertices and $m = |E|$ edges, it holds $M_1(G)/n \leq M_2(G)/m$. This conjecture has been disproved in general graphs and it has

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been proved for chemical graphs and trees in [5, 6]. These indices have been generalized to variable first and second Zagreb indices [4] defined as

$$^{\lambda}M_1(G) = \sum_{v_i \in V} d_i^{2\lambda} \quad \text{and} \quad ^{\lambda}M_2(G) = \sum_{v_i v_j \in E} d_i^{\lambda} \cdot d_j^{\lambda}.$$

The generalization of the above claim to the variable Zagreb indices have been analyzed in [7] and [8]. Namely, it has been analyzed for which λ it holds

$$^{\lambda}M_1(G)/n \leq \ ^{\lambda}M_1(G)/m \ . \tag{1}$$

The following results have been obtained in [7, 8, 9] .

(i) (1) is true for all graphs G and all $\lambda \in [0, 1/2]$,

(ii) (1) is true for all chemical graphs and all $\lambda \in [0, 1]$,

(iii) (1) is true for all trees and all $\lambda \in [0, 1]$.

(iv) (1) is not true for bicyclic graphs and $\lambda = 1$.

Also, it has been proved that for every $\lambda \in R \backslash [0, 1]$ and every complete unbalanced bipartite graphs G, it holds that $^{\lambda}M_1(G)/n > \ ^{\lambda}M_2(G)/m$. In this paper, we will show that $^{\lambda}M_1(G)/n \leq \ ^{\lambda}M_2(G)/m$ holds for all unicyclic graphs and all $\lambda \in [0, 1]$.

2 Main result

Denoted by $h(G) = \ ^{\lambda}M_2(G) - \ ^{\lambda}M_1(G)$. Now we are ready to give the following result which is useful in Theorem 2.3.

Lemma 2.1. *Let G be a connected graph of order n , possessing two adjacent vertices v_i and v_j of degrees $d_i \geq 2$ and $d_j \geq 2$, respectively. Also let a vertex v_k of degree one be attached to a vertex v_l of degree d_l . Let the graph G^* be obtained from G by adding edges $v_i v_k$ and $v_k v_j$ in $G - v_i v_j - v_k v_l$. If $\lambda \in [0, 1]$, then $h(G) \geq h(G^*)$.*

Proof: Now we have

$$ {}^{\lambda}M_1(G^*) - {}^{\lambda}M_1(G) = 2^{2\lambda} + (d_l - 1)^{2\lambda} - d_l^{2\lambda} - 1 \tag{2} $$

and
$$ {}^{\lambda}M_2(G^*) - {}^{\lambda}M_2(G) = 2^{\lambda}(d_i^{\lambda} + d_j^{\lambda}) - d_i^{\lambda} \cdot d_j^{\lambda} - d_l^{\lambda} - (d_l^{\lambda} - (d_l - 1)^{\lambda}) \times \sum_{\substack{v_{l_r}: v_l v_{l_r} \in E \\ l_r \neq k}} {d_{l_r}}^{\lambda} , \tag{3} $$

where d_{l_r} is the degree of vertex v_{l_r}. From (2) and (3) we obtain

$$ \begin{aligned} h(G) - h(G^*) &= {}^{\lambda}M_2(G) - {}^{\lambda}M_2(G^*) - {}^{\lambda}M_1(G) + {}^{\lambda}M_1(G^*) \\ &= 2^{2\lambda} + (d_l - 1)^{2\lambda} - d_l^{2\lambda} - 1 - 2^{\lambda}(d_i^{\lambda} + d_j^{\lambda}) + d_i^{\lambda} \cdot d_j^{\lambda} + d_l^{\lambda} \\ &\qquad + (d_l^{\lambda} - (d_l - 1)^{\lambda}) \sum_{\substack{v_{l_r}: v_l v_{l_r} \in E \\ l_r \neq k}} {d_{l_r}}^{\lambda} \\ &= (d_i^{\lambda} - 2^{\lambda})(d_j^{\lambda} - 2^{\lambda}) + d_l^{\lambda} + (d_l - 1)^{2\lambda} - d_l^{2\lambda} - 1 \\ &\qquad + (d_l^{\lambda} - (d_l - 1)^{\lambda}) \sum_{\substack{v_{l_r}: v_l v_{l_r} \in E \\ l_r \neq k}} {d_{l_r}}^{\lambda} . \end{aligned} \tag{4} $$

Since $d_i, d_j \geq 2$, we have that $(d_i^{\lambda} - 2^{\lambda})(d_j^{\lambda} - 2^{\lambda}) \geq 0$. Therefore, it is sufficient to prove that

$$ d_l^{\lambda} + (d_l - 1)^{2\lambda} - d_l^{2\lambda} - 1 + (d_l^{\lambda} - (d_l - 1)^{\lambda}) \sum_{\substack{v_{l_r}: v_l v_{l_r} \in E \\ l_r \neq k}} {d_{l_r}}^{\lambda} \geq 0 . $$

Since G is connected,

$$ \sum_{\substack{v_{l_r}: v_l v_{l_r} \in E \\ l_r \neq k}} {d_{l_r}}^{\lambda} \geq 2^{\lambda} + d_l - 2 . \tag{5} $$

Hence, it is sufficient to prove that

$$ \begin{aligned} &(d_l^{\lambda} - (d_l - 1)^{\lambda})\Big(\sum_{\substack{v_{l_r}: v_l v_{l_r} \in E \\ l_r \neq k}} {d_{l_r}}^{\lambda} + 1 \Big) + (d_l - 1)^{\lambda} + (d_l - 1)^{2\lambda} - d_l^{2\lambda} - 1 \\ &\qquad \geq (d_l^{\lambda} - (d_l - 1)^{\lambda})(d_l + 2^{\lambda} - 1) + (d_l - 1)^{\lambda} + (d_l - 1)^{2\lambda} - d_l^{2\lambda} - 1 \geq 0 . \end{aligned} \tag{6} $$

Consider the function

$$ \begin{aligned} \varphi(x, \lambda) &= (x^{\lambda} - (x - 1)^{\lambda})(2^{\lambda} + x - x^{\lambda} - (x - 1)^{\lambda} - 1) + (x - 1)^{\lambda} - 1 \\ &= (x^{\lambda} - (x - 1)^{\lambda})(2^{\lambda} + x - x^{\lambda} - (x - 1)^{\lambda} - 2) + x^{\lambda} - 1 \quad \text{for all } x \geq 2 . \end{aligned} \tag{7} $$

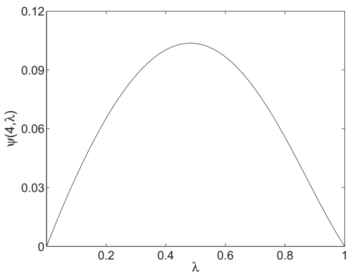

Figure 1.

Using the mean value theorem, we get $x^\lambda - (x-1)^\lambda \geq \lambda x^{\lambda-1}$. The following inequalities are clear.

$$x^\lambda \leq x \quad \text{and} \quad (x-1)^\lambda \leq x-1 \ .$$

If we use above inequalities in (7), then we get

$$\varphi(x,\lambda) \geq \lambda x^{\lambda-1}(2^\lambda - x - 1) + x^\lambda - 1 = \psi(x,\lambda), \quad \text{(say)} \ .$$

Now we have

$$\frac{\partial}{\partial x}\psi(x,\lambda) = \lambda(1-\lambda)x^{\lambda-2}(x+1-2^\lambda) \geq 0\,, \text{ for } x \geq 2\,,\ \lambda \in [0,1]\,.$$

Thus $\psi(x,\lambda)$ is an increasing function for $x \geq 2$. The graph in Figure 1 shows that $\psi(4,\lambda)$ is nonnegative for all $\lambda \in [0,1]$ and hence $\varphi(x,\lambda) \geq 0$ for all $x \geq 4$. One can easily see that $\varphi(3,\lambda) = (3^\lambda - 1)(1 + 2^\lambda - 3^\lambda)$ is a decreasing function in $[0,1]$. Since $\varphi(3,0) = 1$ and $\varphi(3,1) = 0$, we have $\varphi(3,\lambda) \geq 0$. Also we have $\varphi(2,\lambda) = 0$.

Thus $\varphi(x,\lambda) \geq 0$ for all $x \geq 2$ and $\lambda \in [0,1]$, that is, (6) is true and hence the lemma. $\square$

Corollary 2.2. *Let C_n' be a unicyclic graph of order n with cycle of length $n-1$. If $\lambda \in (0,1]$, then $h(C_n') > h(C_n)$.*

Proof: Let v_k be a vertex of degree one is attached a vertex v_l of degree three in $C_n^{'}$. From (5), we get

$$\sum_{\substack{v_{l_r}:v_l v_{l_r}\in E\\ l_r\neq k}} {d_{l_r}}^{\lambda} = 2^{\lambda} + 2^{\lambda} > 2^{\lambda} + 1 \text{ as } \lambda \in (0,1]\ .$$

Thus inequality in (5) is strict and hence $h(C_n^{'}) > h(C_n)$. □

Theorem 2.3. *Let G be a unicyclic graph of order n. Then, ${}^{\lambda}M_2 \geq {}^{\lambda}M_1$ for all $\lambda \in [0,1]$. Moreover, if $\lambda \in (0,1]$, then ${}^{\lambda}M_2 = {}^{\lambda}M_1$ holds if and only if G is isomorphic to C_n, where C_n is a cycle with n vertices.*

Proof: Let C be cycle in unicyclic graph G. Also let two adjacent vertices v_i and v_j be in $V(C)$, where $V(C)$ is the set of vertices in cycle C. The transformation $G \Rightarrow G^*$, described in Lemma 2.1, either decreases the h-value or leaves it unchanged. If $G^* \ncong C_n$, then G^* possess a vertex v_k of degree one. Again we assume that two adjacent vertices v_i and v_j are in cycle of G^*. So one can apply the same transformation to G^*. Repeating the transformation with above construction sufficiently many times we ultimately arrive at C_n. Thus

$$h(G) \geq h(G^*) \geq h(G^{**}) \geq \cdots \geq h(C_n) = 0\ . \tag{8}$$

where C_n is a cycle with n vertices. Thus ${}^{\lambda}M_2(G) \geq {}^{\lambda}M_1(G)$ for all $\lambda \in [0,1]$.

When G is isomorphic to C_n, $h(G) = 0$, that is, ${}^{\lambda}M_2(G) = {}^{\lambda}M_1(G)$. If $\lambda \in (0,1]$ and $G \ncong C_n$, then

$$h(G) \geq h(G^*) \geq h(G^{**}) \geq \cdots \geq h(C_n^{'}) > h(C_n) = 0\,, \text{ by Corollary 2.2,}$$

where $C_n^{'}$ is a unicyclic graph of order n with cycle of length $n-1$. Thus $h(G) > 0$, that is, ${}^{\lambda}M_2(G) > {}^{\lambda}M_1(G)$. Hence ${}^{\lambda}M_2(G) = {}^{\lambda}M_1(G)$ holds if and only if G is isomorphic to C_n. □

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References

[1] S. Nikolić, G. Kovačević, A. Milićević, N. Trinajstić, *The Zagreb indices 30 years after*, Croat. Chem. Acta **76** (2003) 113–124.

[2] I. Gutman, K. C. Das, *The first Zagreb indices 30 years after*, MATCH Commun. Math. Comput. Chem **50** (2004) 83-92.

[3] K. C. Das, I. Gutman, *Some Properties of the Second Zagreb Index*, MATCH Commun. Math. Comput. Chem **52** (2004) 103-112.

[4] A. Milicević, S. Nikolić, On Variable Zagreb Indices, Croat. Chem. Acta **77** (2004) 97-101.

[5] P. Hansen, D. Vukičević, *Comparing the Zagreb indices*, Croat. Chem. Acta **80** (2007) 165-168.

[6] D. Vukičević, A. Graovac, *Comparing Zagreb M1 and M2 indices for acyclic molecules*, MATCH Commun. Math. Comput. Chem **57** (2007) 587-590.

[7] D. Vukičević, *Comparing variable Zagreb indices*, MATCH Commun. Math. Comput. Chem **57** (2007) 633-641.

[8] D. Vukičević, A. Graovac, *Comparing Variable Zagreb M1 and M2 Indices for Acyclic Molecules*, MATCH Commun. Math. Comput. Chem **60** (2008) 37-44.

[9] D. Vukičević, A. Graovac, *Comparing Zagreb M1 and M2 Indices: Overview of the results*, personal communication.