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Direct Comparison of the Variable Zagreb Indices of Cyclic Graphs

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Abstract

Given a graph $G = (V, E)$, the 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. Let $\mathcal{G}_\nu$ be the class of connected graphs with cyclomatic number ν ($\nu \geq 1$). In this paper, we give a lower bound on ${}^{\lambda}M_2(G) - {}^{\lambda}M_1(G)$ in terms of ν and λ in $\mathcal{G}_\nu$ for all $\lambda \in (0, 1]$ and characterize the extremal graphs.

1 Introduction

Let $G = (V, E)$ be a simple connected graph with $|V(G)| = n$ vertices and $|E(G)| = m$ edges. For $v_i \in V(G)$, d_i is the degree of the vertex v_i of graph G, $i = 1, 2, \ldots, n$. The average of the degrees of the vertices adjacent to vertex v_i is denoted by μ_i. A pendant vertex is a vertex of degree one. The cyclomatic number of a connected graph is equal to $\nu = m - n + 1$, i. e., its number of independent cycles. Clearly, $\nu \geq 0$ for all connected graphs. If a graph G has $\nu = 0$, $\nu = 1$ and $\nu = 2$, then it is called tree, unicyclic and

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bicyclic, respectively. We denote the class of connected graphs with cyclomatic number $\nu \geq 1$ by $\mathcal{G}_\nu$.

The vertex independence number of a graph, often called simply "the" independence number, is the cardinality of the largest independent vertex set (no two vertices in the independent set are adjacent), i.e., the size of a maximum independent vertex set. The independence number is most commonly denoted by $\alpha(G)$. Formally,

$$\alpha(G) = \max\{|U| \, : \, U \subset V(G) \;\; \text{independent}\}$$

for a graph G, where $V(G)$ is the vertex set of G and $|U|$ denotes the cardinal number of the set U. The cycle graph with n vertices is called C_n.

The classical first Zagreb index M_1 and second Zagreb index M_2 of graph G (see [6,10, 18–20] and the references therein) are among the oldest and the most famous topological indices and they are defined as

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

Caporossi and Hansen [3, 4] conjectured that, for all connected graphs G it holds that

$$\frac{M_1(G)}{n} \leq \frac{M_2(G)}{m} \tag{1}$$

and the bound is tight for complete graphs.

Although this conjecture is disproved for general graphs [11], it is true for chemical graphs [11], trees [24], unicyclic graphs [16], bicyclic graphs except one class [22], and graphs with small difference between the maximum and minimum vertex degrees [23]. Moreover, it has been shown that for every $\nu \geq 2$, there exists a connected graph in which the inequality (1) does not hold [13] and (1) holds for some special kind of graphs [7, 14]. Nowadays the relation (1) is usually referred to as the Zagreb indices inequality.

The Zagreb indices have been generalized to variable first and second Zagreb indices 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 Zagreb indices inequality to the variable Zagreb indices has been analyzed, namely for which λ it holds that

$$\frac{^{\lambda}M_1(G)}{n} \leq \frac{^{\lambda}M_2(G)}{m} \, , \tag{2}$$

where λ is any real number.

If $\lambda \in [0,1]$ then it is true for chemical graphs [25], trees [26], unicyclic graphs [12], graphs with small difference between the maximum and minimum vertex degrees [17]. If $\lambda \in [0, \sqrt{2}/2]$, then (2) holds for all graphs [1, 2, 25].

Recently, much attention is being paid to the comparison of M_1 and M_2 of graph G. Direct comparisons were obtained on the Zagreb indices for trees [8, 21] and cyclic graphs [5]. Recently, the difference of the classical first and second Zagreb indices of a graph G has been studied in [9, 15] and determined a few basic properties of the reduced second Zagreb index.

The classical Zagreb indices were directly compared in the above mentioned few papers, but the variable Zagreb indices were not directly compared. From this point of view, we characterize the graphs $G \in \mathcal{G}_\nu$ with minimum value of the difference of the variable first and second Zagreb indices for all $\lambda \in (0,1]$ and give a lower bound on ${}^{\lambda}M_2(G) - {}^{\lambda}M_1(G)$ in terms of ν and $\lambda \in (0,1]$.

2 Difference of the variable Zagreb indices of graphs

Let a pendant vertex v_k be adjacent to a vertex v_ℓ of connected graph G, different from the star graph. Then we consider the following inequality

$$\sum_{\substack{v_r:\, v_\ell v_r \in E \\ r \neq k}} d_r^{\lambda} \geq 2^{\lambda} + d_\ell - 2, \quad \text{where} \quad \lambda \in (0,\, 1] \tag{3}$$

which is used in the proof of Lemma 1 of [12]. It is easy to see that if $d_\ell\, \mu_\ell - d_\ell \geq 2$, then the inequality in (3) is strict.

Hence we reformulate the Lemma 1 in [12] as follows.

Lemma 1. *Let $\lambda \in (0,1]$ and G be a connected graph, possessing two adjacent vertices v_i and v_j of degree greater than one. Also let a pendant vertex v_k be adjacent to a vertex v_l. Let the graph G' be obtained from G by adding edges v_iv_k and v_kv_j in $G - v_iv_j - v_kv_l$.*

(i) If $d_\ell\, \mu_\ell - d_\ell = 1$, then

$${}^{\lambda}M_2(G) - {}^{\lambda}M_1(G) \geq {}^{\lambda}M_2(G') - {}^{\lambda}M_1(G').$$

(ii) If $d_\ell\, \mu_\ell - d_\ell \geq 2$, then

$${}^{\lambda}M_2(G) - {}^{\lambda}M_1(G) > {}^{\lambda}M_2(G') - {}^{\lambda}M_1(G').$$

Lemma 2. *Let G be a graph in $\mathcal{G}_\nu$ and $\lambda \in (0,1]$. If ${}^\lambda M_2(G) - {}^\lambda M_1(G)$ is minimum, then G does not contain any pendant vertex.*

Proof. We prove this result by contradiction. For this let G be a graph with at least one pendant vertex in $\mathcal{G}_\nu$ and $\lambda \in (0,1]$ such that ${}^\lambda M_2(G) - {}^\lambda M_1(G)$ is minimum. Let v_k be a pendant vertex that is adjacent to a vertex v_ℓ in G. Also let v_i and v_j be two adjacent vertices in a cycle of G. Then, clearly $d_i \geq 2$ and $d_j \geq 2$. We now apply the transformation considered in Lemma 1 to G. Let the graph G' be obtained from G by adding edges v_iv_k and v_jv_k in $G - v_iv_j - v_kv_\ell$. Then $G' \in \mathcal{G}_\nu$ and by Lemma 1,

$$ {}^\lambda M_2(G) - {}^\lambda M_1(G) \geq {}^\lambda M_2(G') - {}^\lambda M_1(G') \,. $$

If G' contains a pendant vertex, then we repeat the above transformation and non-increase the value ${}^\lambda M_2 - {}^\lambda M_1$. We continue this process and after several times, we can obtain a graph G^{**} in $\mathcal{G}_\nu$ such that $d_i \geq 2$ for all $v_i \in V(G^{**})$. Let G^* be a graph with exactly one pendant vertex in $\mathcal{G}_\nu$ such that

$$ {}^\lambda M_2(G) - {}^\lambda M_1(G) \geq {}^\lambda M_2(G') - {}^\lambda M_1(G') \geq \cdots \geq {}^\lambda M_2(G^*) - {}^\lambda M_1(G^*) \\ \geq {}^\lambda M_2(G^{**}) - {}^\lambda M_1(G^{**}) \,. $$

Thus G^{**} does not contain any pendant vertex and G^* contains exactly one pendant vertex v_r with $v_r\, v_s \in E(G^*)$, (say), such that $d_s\, \mu_s \geq d_s + 2$ for $v_s \in V(G^*)$ (Otherwise, G^{**} contains a pendant vertex, a contradiction). By Lemma 1, we have

$$ {}^\lambda M_2(G^*) - {}^\lambda M_1(G^*) > {}^\lambda M_2(G^{**}) - {}^\lambda M_1(G^{**}) \,. $$

Therefore

$$ {}^\lambda M_2(G) - {}^\lambda M_1(G) > {}^\lambda M_2(G^{**}) - {}^\lambda M_1(G^{**}) \,. $$

This inequality is strict then it contradicts the fact that ${}^\lambda M_2(G) - {}^\lambda M_1(G)$ has minimum value. This completes the proof of the lemma. ■

Lemma 3. *Let G be a graph in $\mathcal{G}_\nu$ and $\lambda \in (0,\, 1]$. Also let ${}^\lambda M_2(G) - {}^\lambda M_1(G)$ be minimum. If $d_i \geq 3$, then $d_j = 2$ for all v_j, $v_i\, v_j \in E(G)$.*

Proof. Once again, we prove this result by contradiction. Assume that there are two adjacent vertices v_i and v_j in G such that $d_i > 2$ and $d_j > 2$. We denote by G' the graph obtained from $G - v_i\, v_j$ by inserting a new vertex v_k such that $v_i\, v_k \in E(G')$ and $v_j\, v_k \in E(G')$. Then clearly $G' \in \mathcal{G}_\nu$ and $d(v_k) = 2$. Therefore, we have

$$ {}^\lambda M_1(G) - {}^\lambda M_1(G') = -2^{2\lambda} \tag{4} $$

and

$$ {}^{\lambda}M_2(G) - {}^{\lambda}M_2(G') = d_i^{\lambda}\, d_j^{\lambda} - 2^{\lambda}\,(d_i^{\lambda} + d_j^{\lambda}). \tag{5} $$

From (4) and (5) we obtain

$$ \begin{aligned} {}^{\lambda}M_2(G) - {}^{\lambda}M_1(G) - \left({}^{\lambda}M_2(G') - {}^{\lambda}M_1(G')\right) &= d_i^{\lambda}\, d_j^{\lambda} - 2^{\lambda}\,(d_i^{\lambda} + d_j^{\lambda}) + 2^{2\lambda} \\ &= (d_i^{\lambda} - 2^{\lambda})(d_j^{\lambda} - 2^{\lambda}) > 0, \end{aligned} $$

since $d_i > 2$, $d_j > 2$ and $\lambda \in (0,\, 1]$. Thus

$$ {}^{\lambda}M_2(G) - {}^{\lambda}M_1(G) >^{\lambda} M_2(G') - {}^{\lambda}M_1(G'). $$

This contradicts the fact that ${}^{\lambda}M_2(G) - {}^{\lambda}M_1(G)$ is minimum. Hence $d_i \leq 2$ or $d_j \leq 2$. By Lemma 2, we have that G does not contain any pendant vertex. Since G is connected, we conclude that $d_i = 2$ and/or $d_j = 2$ for any edge $v_i\, v_j \in E(G)$. This completes the proof. ■

An edge e of a graph G is said to be contracted if it is deleted and its end vertices are identified, the obtained graph is denoted by $G \cdot e$.

Lemma 4. *Let e be an edge with end vertices of degree two in a graph G. Then*

$$ {}^{\lambda}M_2(G) - {}^{\lambda}M_1(G) =^{\lambda} M_2(G \cdot e) - {}^{\lambda}M_1(G \cdot e) \qquad \textit{for all} \;\; \lambda \in R. $$

Proof. By an elementary calculation, we have

$$ {}^{\lambda}M_1(G) - {}^{\lambda}M_1(G \cdot e) = 2^{2\lambda} \quad \text{and} \quad {}^{\lambda}M_2(G) - {}^{\lambda}M_2(G \cdot e) = 2^{2\lambda}\,. $$

From the above results, we get the required result. ■

Lemma 5. *For fixed $\lambda \in (0,\, 1]$,*

$$ f(x,\, \lambda) = x^{\lambda+1}\, 2^{\lambda} - x^{2\lambda} - x\, 2^{2\lambda-1}. $$

Then $f(x,\, \lambda)$ is an increasing function on $x \geq 4$.

Proof. Let us consider a function

$$ g(x,\, \lambda) = (\lambda + 1)\, 2^{\lambda} - 2\lambda\, x^{\lambda-1}. $$

Then $g'(x,\, \lambda) = 2\lambda\,(1-\lambda)\, x^{\lambda-2} \geq 0$ for $x \geq 4$ and hence $g'(x,\, \lambda)$ is an increasing function on $x \geq 4$. Therefore we have

$$ g(x,\, \lambda) \geq g(4,\, \lambda) = (\lambda+1)\, 2^{\lambda} - 2\lambda\, 4^{\lambda-1} = 2^{\lambda}\, \left[\lambda + 1 - \lambda\, 2^{\lambda-1}\right] \geq 2^{\lambda} \geq 1. $$

Since $x \geq 4$, using the above result, we have

$$f'(x,\,\lambda) = x^{\lambda}\,\left[(\lambda+1)\,2^{\lambda} - 2\lambda x^{\lambda-1}\right] - 2^{2\lambda-1} \geq x^{\lambda} - 2^{2\,\lambda-1} \geq 2^{2\,\lambda} - 2^{2\,\lambda-1} > 0.$$

Hence we get the required result. ■

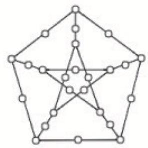

Figure 1. Subdivision of the Petersen graph.

Let Γ be a class of graphs $H = (V,\,E)$ in $\mathcal{G}_{\nu}$ such that $2 \leq d_i \leq 3$ (there exists a vertex v_k in H such that $d_k = 3$) for all $v_i \in V(H)$ and the set of vertices of degree three is an independent set in H. Therefore any graph in Γ is a molecular graph (recall that a connected graph with maximum degree at most 4 belongs to a family of molecular graphs depicting carbon compounds).

It is not difficult to illustrate the graphs in Γ with cyclomatic number ν. The subdivision graph of a graph G is obtained by inserting new vertices of degree two on each edge of G. Hence a subdivision of any 3-regular graph with cyclomatic number ν is in Γ. For example, a subdivision of the Petersen graph is 6-cyclic graph and is in Γ (see Figure 1). We now calculate the difference between the variable Zagreb indices for the graphs G in Γ.

Lemma 6. *Let G be a graph in Γ. Then*

$${}^{\lambda}M_2(G) - {}^{\lambda}M_1(G) = (\nu-1)\,\left(3^{\lambda+1}\,2^{\lambda+1} - 2\cdot 3^{2\lambda} - 3\cdot 2^{2\lambda}\right).$$

Proof. We denote by G_1 the graph obtained from G ($\ncong C_n$) by contracting all edges with end vertices of degree two. Then G_1 contain vertices of degree two and three, and vertices of degree two are adjacent to vertices of degree three. Let k be the number of vertices of degree three in the graph G_1. Therefore the number of vertices of degree two is $3k/2$ as the number of edges in G_1 is $3k$. Moreover, the cyclomatic number of G_1 is ν and by Lemma 4, we have

$${}^{\lambda}M_2(G) - {}^{\lambda}M_1(G) = {}^{\lambda}M_2(G_1) - {}^{\lambda}M_1(G_1)\,.$$

Now,

$$^{\lambda}M_1(G_1) = 3^{2\lambda}\, k + 3 \cdot 2^{2\lambda-1}\, k \quad \text{and} \quad ^{\lambda}M_2(G_1) = 3^{\lambda+1}\, 2^{\lambda}\, k.$$

Since G_1 has $5k/2$ vertices and $3k$ edges, therefore $\nu - 1 = k/2$ for G_1. Thus, we obtain

$$\begin{aligned} ^{\lambda}M_2(G_1) - \, ^{\lambda}M_1(G_1) &= \frac{k}{2}\left(2^{\lambda+1}3^{\lambda+1} - 2 \cdot 3^{2\lambda} - 3 \cdot 2^{2\lambda}\right) \\ &= (\nu - 1)\, \left(3^{\lambda+1}\, 2^{\lambda+1} - 2 \cdot 3^{2\lambda} - 3 \cdot 2^{2\lambda}\right) \; . \end{aligned}$$

From the above, we get the required result. ■

Now we are ready to give a lower bound on $^{\lambda}M_2 - \, ^{\lambda}M_1$ in $\mathcal{G}_{\nu}$ for all $\lambda \in (0, 1]$ and characterize the extremal graphs.

Theorem 1. *Let G be a graph in $\mathcal{G}_{\nu}$ and $\lambda \in (0, 1]$. Then*

$$^{\lambda}M_2(G) - \, ^{\lambda}M_1(G) \geq (\nu - 1)\, \left(3^{\lambda+1}\, 2^{\lambda+1} - 2 \cdot 3^{2\lambda} - 3 \cdot 2^{2\lambda}\right) \tag{6}$$

with equality holding if and only if $G \cong C_n$ or $G \in \Gamma$.

Proof. For $G \cong C_n$, $\nu = 1$ and hence the equality holds in (6). Otherwise, $G \ncong C_n$. Since $G \in \mathcal{G}_{\nu}$, we must have $\Delta \geq 3$. The first variable Zagreb index can also be expressed as

$$^{\lambda}M_1(G) = \sum_{v_i v_j \in E} \left(d_i^{2\lambda-1} + d_j^{2\lambda-1}\right).$$

By Lemma 2, if $^{\lambda}M_2(G) - \, ^{\lambda}M_1(G)$ is minimum, then G has vertices of degree two or more. Again by Lemma 3, if $^{\lambda}M_2(G) - \, ^{\lambda}M_1(G)$ is minimum, then G has for any edge $v_i\, v_j \in E(G)$, $d_i = 2$ or/and $d_j = 2$, that is, the set of vertices of degree greater than 2 (if exists), is an independent set. Therefore, we have

$$\begin{aligned} ^{\lambda}M_2(G) - \, ^{\lambda}M_1(G) &= \sum_{v_i v_j \in E} d_i^{\lambda}\, d_j^{\lambda} - \sum_{v_i v_j \in E} \left(d_i^{2\lambda-1} + d_j^{2\lambda-1}\right) \\ &= \sum_{v_i v_j \in E} \left(d_i^{\lambda}\, d_j^{\lambda} - d_i^{2\lambda-1} - d_j^{2\lambda-1}\right) \\ &\geq \sum_{v_i \in V,\, d_i > 2} d_i\, \left(d_i^{\lambda}\, 2^{\lambda} - d_i^{2\lambda-1} - 2^{2\lambda-1}\right) \end{aligned} \tag{7}$$

because $d_i^{\lambda}\, d_j^{\lambda} - d_i^{2\lambda-1} - d_j^{2\lambda-1} = 0$ for $d_i = d_j = 2$, $v_i v_j \in E$.

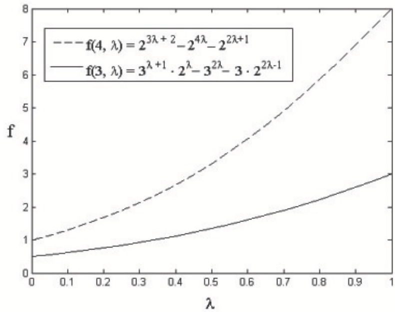

Figure 2. Graphs of two functions.

Consider the function

$$f(x,\,\lambda) = x^{\lambda+1}\,2^{\lambda} - x^{2\lambda} - x\,2^{2\lambda-1}\,, \quad x \geq 3 \quad \text{and} \quad \lambda \in (0,1].$$

By Lemma 5, $f(x,\,\lambda)$ is an increasing function for $x \geq 4$. From Figure 2, one can easily see that $f(4,\,\lambda) > f(3,\,\lambda)$. Hence

$$^{\lambda}M_2(G) - {}^{\lambda}M_1(G) \;\; \geq \;\; \sum_{v_i \in V,\, d_i > 2} \left(3^{\lambda+1}\,2^{\lambda} - 3^{2\lambda} - 3 \cdot 2^{2\lambda-1}\right).$$

Suppose that

$$^{\lambda}M_2(G') - {}^{\lambda}M_1(G') = \sum_{v_i \in V,\, d_i > 2} \left(3^{\lambda+1}\,2^{\lambda} - 3^{2\lambda} - 3 \cdot 2^{2\lambda-1}\right).$$

Let m (m') and n (n') be the number of edges and vertices in G (G'), respectively. Since $G,\, G' \in \mathcal{G}_{\nu}$, we have $\nu - 1 = m - n = m' - n'$. Since G' has vertices of degree 2 and 3, then the number of vertices of degree 3 is exactly $2(m' - n')$ in G'. Then we have

$$\begin{aligned} ^{\lambda}M_2(G) - {}^{\lambda}M_1(G) \;\; &\geq \;\; 2(m'-n')\left(3^{\lambda+1}\,2^{\lambda} - 3^{2\lambda} - 3 \cdot 2^{2\lambda-1}\right) \\ &= \;\; (\nu - 1)\left(3^{\lambda+1}\,2^{\lambda+1} - 2 \cdot 3^{2\lambda} - 3 \cdot 2^{2\lambda}\right). \end{aligned}$$

The first part of the proof is done.

Suppose that equality holds in (6) with $G \not\cong C_n$. By Lemmas 2 and 3 with the above results, we conclude that all the vertices in G have degree 2 or 3 and the set of vertices of degree 3 is an independent set in G, that is, $G \in \Gamma$.

Conversely, one can easily see that the equality holds in (6) for $G \in \Gamma$, by Lemma 6. ■

Finally, note that the main result of [12] and one result of [5] directly follow from Theorem 1 when $\nu = 1$ and $\lambda = 1$, respectively.

Corollary 7. [12] *Let G be a unicyclic graph of order n. For all $\lambda \in (0,1]$, we have* ${}^{\lambda}M_2(G) \geq^{\lambda} M_1(G)$ *with equality holding if and only if $G \cong C_n$.*

Corollary 8. *Let G be a graph in $\mathcal{G}_{\nu}$. Then $M_2(G) - M_1(G) \geq 6(\nu - 1)$ with equality holding if and only if $G \in C_n$ or $G \in \Gamma$.*

Corollary 9. [5] *Let G ($\in \mathcal{G}_{\nu}$) be a graph of order n with m edges. If $n \geq 5(\nu - 1)$, then $M_2(G) - M_1(G) \geq 6(\nu - 1) = 6m - 6n$ with equality holding if and only if $G \in C_n$ or $G \in \Gamma$.*

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