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Comparing the Multiplicative Zagreb Indices

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Abstract

Let G = (V, E) be a simple graph with $n = |V|$ vertices and $m = |E|$ edges. The first and the second Zagreb indices of G are defined as $M_1(G) = \sum_{u \in V} d_u^2 = \sum_{uv \in E}[d_u + d_v]$ and $M_2(G) = \sum_{uv \in E} d_u\, d_v$, respectively, where d_u denotes the degree of vertex u. We compare the multiplicative versions of these indices.

1 Introduction

The first and the second Zagreb indices are among the oldest topological indices [2, 8, 12, 17–19], defined in 1972 by Gutman [10]. These indices have since been used to study molecular complexity, chirality, ZE-isomerism and hetero-systems. In this paper, we are concerned with finite graphs without loops, multiple, or directed edges. Let $G = (V, E)$ be a simple graph with $n = |V|$ vertices and $m = |E|$ edges. The degree of a vertex $v \in V$ is denoted as d_v. The first Zagreb index is defined as the sum of the squares of the degrees of the vertices:

$$M_1(G) = \sum_{v \in V} d_v^2$$

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and the second Zagreb index is defined as the sum of the product of the degrees of adjacent vertices:

$$M_2(G) = \sum_{uv \in E} d_u \, d_v \ .$$

For the sake of simplicity, we often use M_1 and M_2 instead of $M_1(G)$ and $M_2(G)$, respectively. The first Zagreb index can also be expressed as a sum over the edges of G [5, 10]:

$$M_1(G) = \sum_{uv \in E} [d_u + d_v] \ . \tag{1}$$

Gutman [7, 9] has recently proposed to consider the multiplicative variants of Zagreb indices as:

$$\begin{aligned} \Pi_1 = \Pi_1(G) &= \prod_{u \in V} d_u^2 \\ \Pi_2 = \Pi_2(G) &= \prod_{uv \in E} d_u \, d_v \ . \end{aligned} \tag{2}$$

Bearing in mind the identity (1), Eliasi and et. al. [6] considered a new multiplicative version of the first Zagreb index, namely:

$$\Pi_1^* = \Pi_1^*(G) = \prod_{uv \in E(G)} [d_u + d_v] \ . \tag{3}$$

It should be noted that in the general case, the indices $\Pi_1(G)$ and $\Pi_1^*(G)$ assume different values. In this paper we show that these indices have the same value only for cycles.

Comparing the values of these indices on the same graph was one very natural aim, which gave, and still gives, very interesting results and we do it here. For example the next conjecture was proposed [3]:

Conjecture 1. *For all simple graphs G with n vertices and m edges,*

$$\frac{M_1(G)}{n} \leq \frac{M_2(G)}{m} \ . \tag{4}$$

As in [1] is maintained, the inequality (4) holds for trees [15], unicycles graphs [14], and graphs of maximum degree four, so called molecular graphs [11], graphs with only two distinct vertex degrees, but does not hold in general ([1, 11, 13]).

We give a multiplicative version of this conjuncture and solve it.

2 Preliminaries

As usual, the cycle of order n is denoted by C_n, the star of order n is denoted by S_n and the complete graph of order n by K_n. We denote for the sake of simplicity by $m_{i,j}$ the number of edges that connect vertices of degrees i and j in the graph G and by n_k the number of vertices in G of degree k. We have

$$n_i = m_{ii} + \sum_{j\in\mathbb{N}} m_{ij} \tag{5}$$

$$|V(G)| = \sum_{i\in\mathbb{N}} n_i \tag{6}$$

$$|E(G)| = \sum_{i\leq j\in\mathbb{N}} m_{ij}\ . \tag{7}$$

Lemma 2.1. *Let $x, y \in N$ such that $x \neq y$. Then,*

$$\frac{\ln x}{x} + \frac{\ln y}{y} < \frac{\ln x}{y} + \frac{\ln y}{x}\ . \tag{8}$$

Proof: Without loss of generality, we may assume that $x < y$. Note that $x^{y-x} < y^{y-x}$, hence by multiplying both sides by $(xy)^x$, we get $x^y y^x < x^x y^y$ and by applying logarithm, $y\ln x + x\ln y < x\ln x + y\ln x$. Dividing the last inequality by xy, we get (8).

3 Comparing the multiplicative versions of Zagreb indices

In the following theorem we compare between Π_1 and Π_1^*, the two multiplicative versions of the first Zagreb index.

Theorem 3.1. *Let G be a simple connected graphs G of order n. Then*

$$\Pi_1(G) \leq \Pi_1^*(G)\ . \tag{9}$$

The equality holds if and only if $G \cong C_n$.

Proof: By notations in the earlier section we have

$$\begin{aligned}\ln \Pi_1 &= 2\sum_{u\in V(G)} \ln d_u = 2\sum_{i=1}^{n-1} n_i \ln i \\ &= 2\sum_{i=1}^{n-1}\left(\frac{m_{ii}+\sum_{j\in\mathbb{N}} m_{ij}}{i}\right)\ln i \\ &= 2\sum_{i=1}^{n-1}\left(m_{ii}+\sum_{j\in\mathbb{N}} m_{ij}\right)\frac{\ln i}{i} \\ &= 2\sum_{i\le j\in\mathbb{N}} m_{ij}\left(\frac{\ln i}{i}+\frac{\ln j}{j}\right). \qquad (10)\end{aligned}$$

Also

$$\ln \Pi_1^*(G) = \sum_{i\le j\in\mathbb{N}} m_{ij}\ln(i+j). \qquad (11)$$

Therefore, by (10) and (11) we obtain

$$\ln \Pi_1^*(G) - \ln \Pi_1(G) = \sum_{i\le j\in\mathbb{N}} m_{ij}\left[\ln(i+j) - 2\left(\frac{\ln i}{i}+\frac{\ln j}{j}\right)\right]. \qquad (12)$$

Let

$$f(i,j) = \ln(i+j) - 2\left(\frac{\ln i}{i}+\frac{\ln j}{j}\right). \qquad (13)$$

If $i \ge 2$ and $j \ge 2$, then $\frac{1}{2}\ln(i+j) \ge \frac{\ln i}{i}$ and $\frac{1}{2}\ln(i+j) \ge \frac{\ln j}{j}$. Hence $f(i,j) \ge 0$ and by considering (12) we obtain $\Pi_1^*(G) \ge \Pi_1(G)$.

If $j \ge 2$ and $i = 1$, then $\frac{1}{2}\ln(1+j) \ge \frac{\ln j}{j}$. Hence $f(i,j) = f(1,j) \ge 0$ and therefore by (12), $\Pi_1^*(G) \ge \Pi_1(G)$. Note that $f(i,j) = 0$ if and only if $i = j = 2$ or equivalently $G \cong C_n$.

Theorem 3.2. *Let G be a simple connected graph with minimum degree δ. Then*

$$\Pi_2(G) \le \frac{\Pi_1(G)^{\frac{n}{2}-\frac{1}{2}}}{\delta^{n(n-1)-2m}}.$$

The equality holds if and only if there is a vertex $u \in V(G)$, such that for each $v \in V(G)$ if $vu \notin E(G)$, then $d_v = \delta$.

Proof: Let u be a vertex of G and $N(u) = \{v \in V(G) | uv \in E(G)\}$. Then

$$\sum_{v\in N(u)} \ln d_v + \sum_{v\notin N(u)} \ln d_v = \sum_{v\in V(G)} \ln d_v = \frac{1}{2}\ln \Pi_1(G)\ .$$

Therefore

$$\begin{aligned}\sum_{v\in N(u)} \ln d_v &= \frac{1}{2}\ln \Pi_1(G) - \sum_{v\notin N(u)} \ln d_v \\ &\leq \frac{1}{2}\ln \Pi_1(G) - \ln d_u - (n-1-d_u)\ln(\delta)\ .\end{aligned}$$

Hence

$$\begin{aligned}\sum_{u\in V(G)}\sum_{v\in N(u)} \ln d_v &\leq \sum_{u\in V(G)} \frac{1}{2}\ln \Pi_1(G) - \sum_{u\in V(G)} \ln d_u - \sum_{u\in V(G)} (n-1-d_u)\ln(\delta) \\ &= \left(\frac{n}{2}-\frac{1}{2}\right)\ln \Pi_1 - n(n-1)\ln(\delta) + 2m\ln(\delta)\ . \qquad (14)\end{aligned}$$

But

$$\begin{aligned}\ln \Pi_2(G) &= \sum_{uv\in E(G)} [\ln d_u + \ln d_v] \\ &= \frac{1}{2}\sum_{u\in V(G)}\sum_{v\in N(U)} [\ln d_u + \ln d_v] \\ &= \frac{1}{2}\sum_{u\in V(G)}\sum_{v\in N(U)} \ln d_u + \frac{1}{2}\sum_{u\in V(G)}\sum_{v\in N(U)} \ln d_v\ .\end{aligned}$$

Therefore

$$\ln \Pi_2(G) = \sum_{u\in V(G)} d_u \ln d_u = \sum_{u\in V(G)}\sum_{v\in N(U)} \ln d_v\ . \qquad (15)$$

By (14) and (15) we obtain

$$\Pi_2(G) \leq \frac{\Pi_1(G)^{\frac{n}{2}-\frac{1}{2}}}{\delta^{n(n-1)-2m}}\ .$$

The equality holds if and only if there is a vertex $u \in V(G)$, such that for each $v \in V(G)$ if $vu \notin E(G)$, then $d_v = \delta$.

Theorem 3.3. *Let G be a graph with m edges. Then*

$$\sqrt{\Pi_2(G)} \leq \frac{\Pi_1^*(G)}{2^m}\ .$$

Moreover, equality holds only for regular graphs.

Proof: We have

$$\frac{\sqrt{\Pi_2(G)}}{\Pi_1^*(G)} = \frac{\prod_{uv\in E(G)}\sqrt{d_u\,d_v}}{2^m\prod_{uv\in E(G)}\frac{d_u+d_v}{2}} = \frac{1}{2^m}\prod_{uv\in E(G)}\frac{\sqrt{d_u\,d_v}}{\frac{d_u+d_v}{2}} \leq \frac{1}{2^m}\ . \qquad (16)$$

In (16) the equality holds if and only if for each edge $uv \in E(G)$, $d_u = d_v$ and thus G is a regular graph.

Theorem 3.4. *Let G be a graph with m edges, maximum degree Δ and minimum degree δ, respectively. Then*

$$\sqrt{\Pi_2(G)} \geq \Pi_1^*(G) \left(\frac{\sqrt{\Delta\delta}}{\Delta+\delta} \right)^m .$$

The equality holds if and only if for every edge of G, its end vertices have degrees Δ and δ.

Proof: For any edge uv of G, assume that $d_u \leq d_v$. Then

$$\frac{\sqrt{\Pi_2(G)}}{\Pi_1^*(G)} = \frac{1}{2^m} \prod_{uv \in E(G)} \frac{2\sqrt{d_u\, d_v}}{[d_u + d_v]} = \frac{1}{2^m} \prod_{uv \in E(G)} f(d_u/d_v) \tag{17}$$

where $f(x) = \frac{2\sqrt{x}}{1+x}$. This function is increasing for $\frac{1}{n+1} \leq x \leq 1$. Note $f(\frac{d_u}{d_v}) \geq f(\frac{\delta}{\Delta}) = \frac{2\sqrt{\Delta\delta}}{\Delta+\delta}$, with equality if and only if $d_u = \delta$ and $d_v = \Delta$. This and equation (17) complete the proof.

Corollary 3.5. *Let G be a graph with n vertices and m edges. Then*

$$\sqrt{\Pi_2(G)} \geq \Pi_1^*(G) \left(\frac{\sqrt{n-1}}{n} \right)^m .$$

The equality holds if and only if G is the star.

Theorem 3.6. *Let G be a molecular graph, i.e $\Delta(G) \leq 4$. Then*

$$\Pi_1^*(G)^4 \geq \Pi_2(G)^3.$$

Proof: Let $g(x,y) = (x+y)^4 - (xy)^3$. Then for each $x, y \in \{1,2,3,4\}$ we have $g(x,y) \geq 0$. Therefore $(x+y)^4 \geq (xy)^3$. Since G is a molecular graph, for each $u \in V(G)$ we have $d_u \in \{1,2,3,4\}$. Hence

$$\prod_{uv \in E(G)} (d_u + d_v)^4 \geq \prod_{uv \in E(G)} (d_u\, d_v)^3$$

and thus

$$\Pi_1^*(G)^4 \geq \Pi_2(G)^3 .$$

The result follows.

Let $G = K_{2,3}$. Then $\sqrt[|V(G)|]{\Pi_1^*(G)} = 6.898$, $\sqrt[|V(G)|]{\Pi_1(G)} = 5.53$ and $\sqrt[|E(G)|]{\Pi_2(G)} = 6$. So $\sqrt[|V(G)|]{\Pi_1^*(G)} \geq \sqrt[|E(G)|]{\Pi_2(G)} \geq \sqrt[|V(G)|]{\Pi_1(G)}$.

Now let $H = P_5$. Then $\sqrt[|V(H)|]{\Pi_1^*(H)} = 2.7$, $\sqrt[|V(H)|]{\Pi_1(H)} = 2.29$ and $\sqrt[|E(H)|]{\Pi_2(H)} = 2.8$. So $\sqrt[|E(H)|]{\Pi_2(H)} \geq \sqrt[|V(H)|]{\Pi_1^*(H)} \geq \sqrt[|V(H)|]{\Pi_1(H)}$.

Now we consider the following theorem that is multiplicative version of Conjecture (1).

Theorem 3.7. *Let G be a graph with n vertices and m edges. Then*

$$\sqrt[n]{\prod_{u \in V} d_u^2} \leq \sqrt[m]{\prod_{uv \in E} d_u\, d_v}\ .$$

Moreover, equality holds only for regular graphs.

Proof: Note that the following sequence of the relations is equivalent:

$$\sqrt[n]{\prod_{u \in V} d_u^2} \leq \sqrt[n]{\prod_{uv \in E} d_u\, d_v}$$

$$\ln \sqrt[n]{\prod_{u \in V} d_u^2} \leq \ln \sqrt[m]{\prod_{uv \in E} d_u\, d_v}$$

$$\frac{\sum_{u \in V} 2 \ln d_u}{n} \leq \frac{\sum_{uv \in E} (\ln d_u + \ln d_v)}{m}$$

$$\frac{\sum_{uv \in E} \left(\frac{2 \ln d_u}{d_u} + \frac{2 \ln d_v}{d_v} \right)}{\sum_{uv \in E} \left(\frac{1}{d_u} + \frac{1}{d_v} \right)} \leq \frac{\sum_{uv \in E} (\ln d_u + \ln d_v)}{\sum_{uv \in E} 1}$$

$$\sum_{uv \in E} \left(\frac{2 \ln d_u}{d_u} + \frac{2 \ln d_v}{d_v} \right) \cdot \sum_{pq \in E} 1 - \sum_{uv \in E} \left(\frac{1}{d_u} + \frac{1}{d_v} \right) \sum_{pq \in E} (\ln d_p + \ln d_q) \leq 0$$

$$\sum_{uv \in E} \sum_{pq \in E} \left(\frac{2 \ln d_u}{d_u} + \frac{2 \ln d_v}{d_v} - \left(\frac{1}{d_u} + \frac{1}{d_v} \right) (\ln d_p + \ln d_q) \right) \leq 0$$

$$\sum_{\{uv, pq\} \in \binom{E}{2}} \left[\frac{2 \ln d_u}{d_u} + \frac{2 \ln d_v}{d_v} - \left(\frac{1}{d_u} + \frac{1}{d_v} \right) (\ln d_p + \ln d_q) + \frac{2 \ln d_p}{d_p} \right.$$

$$\left. + \frac{2 \ln d_q}{d_q - (1/d_p + 1/d_q) (\ln d_u + \ln d_v)} \right] + \sum_{uv \in E} \left[\frac{2 \ln d_u}{d_u} + \frac{2 \ln d_v}{d_v} \right.$$

$$\left. - \left(\frac{1}{d_u} + \frac{1}{d_v} \right) (\ln d_u + \ln d_v) \right] \leq 0$$

$$\sum_{\{uv,pq\}\in\binom{E}{2}} \left[\left(\frac{\ln d_u}{d_u}+\frac{\ln d_p}{d_p}\right)-\left(\frac{\ln d_u}{d_p}+\frac{\ln d_p}{d_u}\right)\right]+\left[\left(\frac{\ln d_v}{d_v}+\frac{\ln d_p}{d_p}\right)-\left(\frac{\ln d_v}{d_p}+\frac{\ln d_p}{d_v}\right)\right]$$

$$+\left[\left(\frac{\ln d_u}{d_u}+\frac{\ln d_q}{d_q}\right)-\left(\frac{\ln d_u}{d_q}+\frac{\ln d_q}{d_u}\right)\right]+\left[\left(\frac{\ln d_v}{d_v}+\frac{\ln d_q}{d_q}\right)-\left(\frac{\ln d_v}{d_q}+\frac{\ln d_q}{d_v}\right)\right]$$

$$+\sum_{uv\in E}\left[\left(\frac{\ln d_u}{d_u}+\frac{\ln d_v}{d_v}\right)-\left(\frac{\ln d_u}{v}+\frac{\ln d_v}{u}\right)\right]\leq 0\ .$$

The last inequality follows form Lemma (2.1) and equality holds only when $u = v = p = q$ for all summands in the first sum and $u = v$ for all summands in the second sum, i. e., when the graph is regular.

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