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RELATIONS BETWEEN ORDINARY AND MULTIPLICATIVE ZAGREB INDICES

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Abstract. The first and second multiplicative Zagreb indices of a graph G are $\Pi_1(G) = \sum\limits_{x\in V(G)} d(x)^2$ and $\Pi_2(G) = \sum\limits_{(x,y)\in E(G)} d(x)\, d(y)$, respectively, where $d(x)$ is the degree of the vertex x. We provide lower and upper bounds for Π_1 and Π_2 of a connected graph in terms of the number of vertices, number of edges, and the ordinary, additive Zagreb indices M_1 and M_2.

1. Introduction

We consider only finite connected graphs without loops and multiple edges. For a connected graph G, by $V(G)$ and $E(G)$ we denote the set of vertices and edges. The numbers of vertices and edges of G are $n = |V(G)|$ and $m = |E(G)|$, respectively. An edge of G connecting the vertices x and y is denoted by (x, y). In order to avoid trivialities, we always assume that $n \geqslant 3$.

The degree $d(x)$ of a vertex x is the number of edges adjacent to x. A vertex x is said to be an r-vertex if its degree is equal to r. The number of r-vertices in G is denoted by n_r. The average degree of a connected graph G is given as $2m/n$.

A graph is said to be regular if all its vertices have mutually equal degrees. If this vertex degree is equal to R, then the graph is said to be R-regular. The degree–based graph invariants M_1 and M_2, called Zagreb indices, were introduced more than thirty years ago by Trinajstić and one of the present authors [**9**]. For their main properties, chemical applications, and further references see [**1**,**7**,**17**,**21**].

The first Zagreb index $M_1(G)$ is equal to the sum of squares of the degrees of the vertices, and the second Zagreb index $M_2(G)$ is equal to the sum of products

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of the degrees of pairs of adjacent vertices of the graph G. It is known that

$$M_1(G) = \sum_{x\in V(G)} d(x)^2 = \sum_{(x,y)\in E(G)} [d(x)+d(y)] = \sum_r \sum_{s\leqslant r} (r+s)\, m_{r,s} \tag{1.1}$$

and

$$M_2(G) = \sum_{(x,y)\in E(G)} d(x)\, d(y) = \sum_r \sum_{s\leqslant r} rs\, m_{r,s} \tag{1.2}$$

where $m_{r,s}$ is the number of edges in G with end-vertex degrees r and s.

In two recent works, Todeschini et al. [**18**, **19**] proposed that multiplicative variants of molecular structure descriptors be considered. When this idea is applied to Zagreb indices, one arrives at their multiplicative versions Π_1 and Π_2, defined as

$$\Pi_1(G) = \prod_{x\in V(G)} d(x)^2 \tag{1.3}$$

$$\Pi_2(G) = \prod_{(x,y)\in E(G)} d(x)\, d(y)\ . \tag{1.4}$$

In a series of recently produced papers [**3**, **5**, **12**, **15**, **22**, **23**], some basic properties of the multiplicative Zagreb indices were established. In connection with this, it should be mentioned that already in the 1980s, Narumi and Katayama [**16**] conceived a simple degree–based multiplicative structure descriptor $NK(G) = \prod_{x\in V(G)} d(x)$, which nowadays is referred to as the "Narumi–Katayama index". This index was studied in [**20**] and recently also in [**8**, **13**, **14**]. Evidently, $\Pi_1(G)$ is just the square of $NK(G)$.

2. An alternative formulation of first and second multiplicative Zagreb indices

LEMMA 2.1. [**2**] *Let f be a non-negative function defined on the set of positive real numbers. Then the graph invariant $T(G)$ can be rewritten in the following form:*

$$T(G) = \sum_{x\in V(G)} f(d(x)) = \sum_{(x,y)\in E(G)} \left(\frac{f(d(x))}{d(x)} + \frac{f(d(y))}{d(y)} \right)$$

$$= \sum_r \sum_{s\leqslant r} \left(\frac{f(r)}{r} + \frac{f(s)}{s} \right)\ . \tag{2.1}$$

PROPOSITION 2.1. *Let G be a connected graph. Then*

$$\Pi_1(G) = \exp\left\{ \sum_{(x,y)\in E(G)} \left(\frac{\ln(d(x)^2)}{d(x)} + \frac{\ln(d(y)^2)}{d(y)} \right) \right\} \tag{2.2}$$

and

$$\Pi_1(G) = \exp\left\{ 2 \sum_r \sum_{s \leqslant r} \left(\frac{\ln(r)}{r} + \frac{\ln(s)}{s} \right) m_{r,s} \right\} . \tag{2.3}$$

PROOF. Defining the function $f(d) = \ln(d^2)$, Eqs. (2.2) and (2.3) follow from (1.3) and the identity (2.1). It is worth noting that if x is a pendent vertex, then $\ln(d(x)) = 0$. □

PROPOSITION 2.2. *The second multiplicative Zagreb index can be reformulated as*

$$\Pi_2(G) = \exp\left\{ \sum_{x \in V(G)} d(x)\, \ln(d(x)) \right\} . \tag{2.4}$$

PROOF. Define the function $f(d) = d \ln(d)$ and apply Lemma 2.1, taking into account Eq. (1.4). □

COROLLARY 2.1. *If the connected graphs G_1 and G_2 are characterized by the same vertex degree distribution $(n_1, n_2, \ldots, n_r, \ldots)$, then not only the indices M_1, Π_1, and NK will be identical for G_1 and G_2, but the equality $\Pi_2(G_1) = \Pi_2(G_2)$ will hold as well.*

PROPOSITION 2.3. *Let G be a connected graph. Then $\Pi_2(G) \geqslant \Pi_1(G)$, and the equality holds if and only if G is a path P_n or a cycle C_n on $n \geqslant 3$ vertices.*

PROOF. Comparing the first and second multiplicative Zagreb indices, we have

$$\begin{aligned} \ln \frac{\Pi_2(G)}{\Pi_1(G)} &= \sum_{x \in V(G)} d(x)\, \ln(d(x)) - \sum_{x \in V(G)} 2 \ln(d(x)) \\ &= n_3 \ln 3 + 2\, n_4 \ln 4 + 3\, n_5 \ln 5 + \cdots \geqslant 0 . \end{aligned}$$

This implies the claim. □

COROLLARY 2.2. *For a hexagonal system H (that possesses only vertices of degree 2 or 3), the number of vertices of degree 3 is $n_3 = 2(h-1)$, where h is the number of hexagons [**6**]. It follows that*

$$\frac{\Pi_2(H)}{\Pi_1(H)} = \exp[n_3 \ln 3] = \exp\left[\ln\left(3^{2(h-1)}\right)\right] = 9^{h-1} .$$

REMARK 2.1. (an interesting analogy) The molecular graphs of phenylenes and their hexagonal squeezes possess only vertices of degree 2 and 3 [**4**]. Denote by $NK(PH)$ and $NK(HS)$ the Narumi–Katayama indices of a phenylene PH and its hexagonal squeeze HS. It was shown [**20**] that $NK(PH)/NK(HS) = 9^{h-1}$.

3. Inequalities for first and second multiplicative Zagreb indices

PROPOSITION 3.1. *Let G be a connected graph. Then*

$$\Pi_1(G) \leqslant \left(\frac{2m}{n}\right)^{2n} .$$

with equality if and only if G is regular.

PROOF. Let P be an arbitrary positive number. Using the inequality between the arithmetic and the geometric mean we get

$$\frac{1}{n}\sum_{x\in V(G)} d(x) \geqslant \left(\prod_{x\in V(G)} d(x)\right)^{1/n} = \exp\left[\frac{1}{nP}\sum_{x\in V(G)} \ln\left(d(x)^P\right)\right]$$

from which it follows

$$\ln\left(\frac{2m}{n}\right) \geqslant \frac{1}{nP}\sum_{x\in V(G)} \ln\left(d(x)^P\right) = \ln\left(\prod_{x\in V(G)} d(x)^P\right)^{1/(nP)}$$

and

$$\prod_{x\in V(G)} d(x)^P \leqslant \left(\frac{2m}{n}\right)^{Pn} .$$

For the case of $P = 2$, the claim follows. □

COROLLARY 3.1. *If $P = 1$, for the Narumi–Katayama index one obtains:*

$$NK(G) \leqslant \left(\frac{2m}{n}\right)^{n}$$

with equality if and only if G is regular.

COROLLARY 3.2. *Because $2m/n$ is the average vertex degree, and $d(x) \leqslant n-1$, for any connected graph G with n vertices*

$$\Pi_1(G) \leqslant \Pi_1(K_n) = (n-1)^{2n} \qquad \text{and} \qquad NK(G) \leqslant NK(K_n) = (n-1)^n .$$

Equality is attained if and only if $G \cong K_n$.

The following lemma is the classical Jensen inequality [**10**]:

LEMMA 3.1. *Let Φ be a real function defined on the interval $(0,\infty)$, and let a_i , $i = 1, 2, \dots, N$, be positive numbers. Let the functions $B(a_1, a_2, \dots, a_N)$ and $C(a_1, a_2, \dots, a_N)$ be defined as*

$$B(a_1, a_2, \dots, a_N) = \Phi\left(\frac{a_1 + a_2 + \cdots + a_N}{N}\right)$$

and

$$C(a_1, a_2, \dots, a_N) = \frac{\Phi(a_1) + \Phi(a_2) + \cdots \Phi(a_N)}{N} .$$

Then $C(a_1, a_2, \dots, a_N) \geqslant B(a_1, a_2, \dots, a_N)$ if Φ is a convex function. If Φ is concave, then the inequality is reversed, i. e., $C(a_1, a_2, \dots, a_N) \leqslant B(a_1, a_2, \dots, a_N)$. Moreover, equality is attained if and only if all a_i are mutually equal.

PROPOSITION 3.2. *Let G be a connected graph. Then*

$$\Pi_1(G) \leqslant \left(\frac{M_1(G)}{n}\right)^n$$

with equality if and only if G is regular.

PROOF. The function $\Phi(d) = \ln(d^2)$ is a strictly concave on the interval $(0, \infty)$, because its second derivative, $\Phi'' = -4/d^2$, is negative. Assuming that $N = n$ and that the positive numbers a_i are the squares of degrees of the vertices, from Lemma 3.1 one obtains

$$\ln\left(\frac{1}{n}\sum_{x\in V(G)} d(x)^2\right) \geqslant \frac{1}{n}\sum_{x\in V(G)} \ln\left(d(x)^2\right) = \frac{1}{n}\ln\left(\prod_{x\in V(G)} d(x)^2\right)$$

i. e.,

$$\ln\left(\frac{M_1(G)}{n}\right) \geqslant \frac{1}{n}\sum_{x\in V(G)} \ln\left(d(x)^2\right) = \ln\left(\prod_{x\in V(G)} d(x)^2\right)^{1/n} .$$

Because the function $\Phi(d) = \ln(d^2)$ is strictly concave, equality holds if and only if the graph G is regular. □

PROPOSITION 3.3. *Let G be a connected graph. Then*

$$\Pi_2(G) \geqslant \left(\frac{2m}{n}\right)^{2m}$$

with equality if and only if G is regular.

PROOF. $\Phi(d) = d\ln(d)$ is a strictly convex function on the interval $(0, \infty)$, because its second derivative, $\Phi'' = 1/d$, is positive. Assuming that $N = n$ and that the positive constants a_i , $i = 1, 2, \ldots, n$, are the degrees of the vertices, from Lemma 3.1 we get

$$\sum_{x\in V(G)} d(x)\ln(d(x)) \geqslant \left(\sum_{x\in V(G)} d(x)\right)\ln\left(\frac{\sum\limits_{x\in V(G)} d(x)}{n}\right) = 2m\ln\left(\frac{2m}{n}\right)$$

implying

$$\ln\left(\prod_{x\in V(G)} d(x)\ln(d(x))\right) \geqslant \ln\left(\frac{2m}{n}\right)^{2m} .$$

Because $\Phi(d) = d\ln(d)$ is a strictly convex function, equality holds if and only if the graph G is regular. □

COROLLARY 3.3. *If G is a unicyclic graph, then $n = m$. Then $\Pi_2(G) \geqslant 4^n$, with equality if and only if G is a cycle C_n on $n \geqslant 3$ vertices.*

Corollary 3.4. *For any connected graph G with n vertices,*

$$\Pi_2(G) \leqslant \Pi_2(K_n) = (n-1)^{n(n-1)} \ .$$

Equality is attained if and only if $G \cong K_n$.

Lemma 3.2. *(* [**11**]) Let G be a connected graph with m edges. Then

$$m \, \ln\left(\frac{M_2(G)}{m}\right) \geqslant \sum_{x \in V(G)} d(x) \, \ln(d(x))$$

with equality if and only if the graph G is regular.

A direct consequence of Lemma 3.2 is:

Proposition 3.4. *Let G be a connected graph. Then*

$$\Pi_2(G) = \exp\left(\sum_{x \in V(G)} d(x) \, \ln(d(x))\right) \leqslant \left(\frac{M_2(G)}{m}\right)^m$$

with equality if and only if G is regular.

4. Chemical graphs

Let G be a chemical graph, namely a graph with vertex degree set $D(G) = \{1, 2, 3, 4\}$. To avoid the trivialities, we assume that the condition $n_3 + n_4 > 0$ holds. Then the following relations hold:

$$\begin{aligned} 2m - n &= n_2 + 2\,n_3 + 3\,n_4 \\ M_1 - n &= 3\,n_2 + 8\,n_3 + 15\,n_4 \\ \ln(\Pi_2/\Pi_1) &= n_3 \, \ln 3 + n_4 \, \ln 16 \ . \end{aligned}$$

The determinant $Det(1)$ of this linear system is equal to $\ln(256/729) < 0$. Consequently, the three unknown variables n_2 , n_3 , and n_4 can be computed as: $n_2 = Det(2)/Det(1)$, $n_3 = Det(3)/Det(1)$ and $n_4 = Det(4)/Det(1)$, where

$$\begin{aligned} Det(2) &= (2m-n)(16 \, \ln 4 - 15 \, \ln 3) + (M_1 - n)(3 \, \ln 3 - 4 \, \ln 4) \\ &+ \ 6 \, \ln(\Pi_2/\Pi_1) \leqslant 0 \\ Det(3) &= (M_1 + 2n - 6m) \, \ln 16 - 6 \, \ln(\Pi_2/\Pi_1) \leqslant 0 \\ Det(4) &= 2 \, \ln(\Pi_2/\Pi_1) - (M_1 + 2n - 6m) \, \ln 3 \leqslant 0 \, . \end{aligned}$$

This immediately implies:

Proposition 4.1. *Let G be a chemical graph with n vertices and m edges, whose first Zagreb index is M_1 . Then*

$$\ln \frac{\Pi_2(G)}{\Pi_1(G)} \leqslant \frac{1}{6} \Big[(M_1 - n)(4 \, \ln 4 - 3 \, \ln 3) - (2m - n)(16 \, \ln 4 - 15 \, \ln 3)\Big]$$

with equality if $n_2 = 0$.

$$\ln \frac{\Pi_2(G)}{\Pi_1(G)} \geqslant \frac{1}{3} \, (M_1 + 2n - 6m) \, \ln 4$$

with equality if $n_3 = 0$.

$$\ln \frac{\Pi_2(G)}{\Pi_1(G)} \leqslant \frac{1}{2}\,(M_1 + 2n - 6m)\,\ln 3$$

with equality if $n_4 = 0$.

For a number of important chemical graphs the vertex degree set $D(G) = \{2, 3\}$ (see [**4**, **6**]). For such graphs we have:

Corollary 4.1. *If the graph G has only vertices of degree 2 and 3, then*

$$\ln \frac{\Pi_2(G)}{\Pi_1(G)} = \frac{1}{2}\,(M_1 + 2n - 6m)\,\ln 3\ .$$

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