RELATIONS BETWEEN ORDINARY AND MULTIPLICATIVE ZAGREB INDICES

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Abstract. The first and second multiplicative Zagreb indices of a graph \( G \) are
\[
\Pi_1(G) = \sum_{x \in V(G)} d(x)^2 \quad \text{and} \quad \Pi_2(G) = \sum_{(x,y) \in E(G)} d(x) d(y),
\]
respectively, where \( d(x) \) is the degree of the vertex \( x \). We provide lower and upper bounds for \( \Pi_1 \) and \( \Pi_2 \) 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 \( n \geq 3 \).

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...
of the degrees of pairs of adjacent vertices of the graph \( G \). It is known that
\[
(1.1) \quad M_1(G) = \sum_{x \in V(G)} d(x)^2 = \sum_{(x,y) \in E(G)} [d(x) + d(y)] = \sum_{r \leq s} (r + s) m_{r,s}
\]
and
\[
(1.2) \quad M_2(G) = \sum_{(x,y) \in E(G)} d(x) d(y) = \sum_{r \leq s} rs m_{r,s},
\]
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. \cite{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 \( \Pi_1 \) and \( \Pi_2 \), defined as
\[
(1.3) \quad \Pi_1(G) = \prod_{x \in V(G)} d(x)^2
\]
\[
(1.4) \quad \Pi_2(G) = \prod_{(x,y) \in E(G)} d(x) d(y).
\]

In a series of recently produced papers \cite{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 \cite{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 \cite{20} and recently also in \cite{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. \cite{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:
\[
T(G) = \sum_{x \in V(G)} f(d(x)) = \sum_{(x,y) \in E(G)} \left( \frac{f(d(x))}{d(x)} + \frac{f(d(y))}{d(y)} \right)
\]
\[
= \sum_{r \leq s} \sum_{r \leq s} \left( \frac{f(r)}{r} + \frac{f(s)}{s} \right).
\]

Proposition 2.1. Let \( G \) be a connected graph. Then
\[
(2.2) \quad \Pi_1(G) = \exp \left\{ \sum_{(x,y) \in E(G)} \left( \ln \frac{d(x)^2}{d(x)} + \ln \frac{d(y)^2}{d(y)} \right) \right\}
\]
and

\[
\Pi_1(G) = \exp \left\{ 2 \sum_{r,s \leq r} \left( \frac{\ln(r)}{r} + \frac{\ln(s)}{s} \right) m_{r,s} \right\}.
\]

**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

\[
\Pi_2(G) = \exp \left\{ \sum_{x \in V(G)} d(x) \ln(d(x)) \right\}.
\]

**Proof.** Define the function \( f(d) = d \ln(d) \) and apply Lemma 2.1, taking into account Eq. (1.4). \( \square \)

**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 \( M_1 \), \( \Pi_1 \), 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 \( \Pi_2(G) \geq \Pi_1(G) \), and the equality holds if and only if \( G \) is a path \( P_n \) or a cycle \( C_n \) on \( n \geq 3 \) vertices.

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

\[
\ln \frac{\Pi_2(G)}{\Pi_1(G)} = \sum_{x \in V(G)} d(x) \ln(d(x)) - \sum_{x \in V(G)} 2 \ln(d(x))
\]

\[
= n_3 \ln 3 + 2 n_4 \ln 4 + 3 n_5 \ln 5 + \cdots \geq 0.
\]

This implies the claim. \( \square \)

**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

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

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

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

from which it follows

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

and

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

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

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

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

with equality if and only if $G$ is regular.

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

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

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

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

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

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

and

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

Then $C(a_1, a_2, \ldots, a_N) \geq B(a_1, a_2, \ldots, a_N)$ if $\Phi$ is a convex function. If $\Phi$ is concave, then the inequality is reversed, i.e., $C(a_1, a_2, \ldots, a_N) \leq B(a_1, a_2, \ldots, a_N)$. Moreover, equality is attained if and only if all $a_i$ are mutually equal.
Proposition 3.2. Let $G$ be a connected graph. Then

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

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

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

i.e.,

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

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

Proposition 3.3. Let $G$ be a connected graph. Then

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

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

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

implying

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

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

Corollary 3.3. If $G$ is a unicyclic graph, then $n = m$. Then $\Pi_2(G) \geq 4^n$, with equality if and only if $G$ is a cycle $C_n$ on $n \geq 3$ vertices.
Corollary 3.4. For any connected graph $G$ with $n$ vertices,
\[ \Pi_2(G) \leq \Pi_2(K_n) = (n-1)^{n(n-1)}. \]
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
\[ m \ln \left( \frac{M_2(G)}{m} \right) \geq \sum_{x \in V(G)} d(x) \ln(d(x)) \]
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
\[ \Pi_2(G) = \exp \left( \sum_{x \in V(G)} d(x) \ln(d(x)) \right) \leq \left( \frac{M_2(G)}{m} \right)^m \]
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:
\[ 2m - n = n_2 + 2n_3 + 3n_4 \]
\[ M_1 - n = 3n_2 + 8n_3 + 15n_4 \]
\[ \ln(\Pi_2/\Pi_1) = n_3 \ln 3 + n_4 \ln 16. \]

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:
\[ n_2 = Det(2)/Det(1), \]
\[ n_3 = Det(3)/Det(1) \text{ and } n_4 = Det(4)/Det(1), \]
where
\[ Det(2) = (2m - n)(16 \ln 4 - 15 \ln 3) + (M_1 - n)(3 \ln 3 - 4 \ln 4) \]
\[ + 6 \ln(\Pi_2/\Pi_1) \leq 0 \]
\[ Det(3) = (M_1 + 2n - 6m) \ln 16 - 6 \ln(\Pi_2/\Pi_1) \leq 0 \]
\[ Det(4) = 2 \ln(\Pi_2/\Pi_1) - (M_1 + 2n - 6m) \ln 3 \leq 0. \]

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
\[ \ln \frac{\Pi_2(G)}{\Pi_1(G)} \leq \frac{1}{6} \left( (M_1 - n)(4 \ln 4 - 3 \ln 3) - (2m - n)(16 \ln 4 - 15 \ln 3) \right) \]
with equality if $n_2 = 0$.

\[ \ln \frac{\Pi_2(G)}{\Pi_1(G)} \geq \frac{1}{3} (M_1 + 2n - 6m) \ln 4 \]
with equality if $n_3 = 0$.

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

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

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

References


(Received by editors 05.06.2012; in revised form 08.06.2012; available on internet 30.06.2012)

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