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Some Observations on Comparing Zagreb Indices

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Abstract

Let G be a simple graph possessing n vertices and m edges. Let d_i be the degree of the i-th vertex of G , $i = 1, \ldots, n$. The first Zagreb index M_1 is the sum of d_i^2 over all vertices of G. The second Zagreb index M_2 is the sum $d_i\, d_j$ over pairs of adjacent vertices of G. In this paper we search for graph for which $M_1/n = M_2/m$, and show how numerous such graphs can be constructed. In addition, we find examples of graphs for which $M_1/n > M_2/m$, which are counterexamples for the earlier conjectured inequality $M_1/n \le M_2/m$.

1. Introduction

Of the countless graph–based molecular structure descriptors, currently used in mathematical chemistry [1–3], quite a few are defined by means of vertex degrees. Of these, the Randić connectivity index [4]

$$R(G) = \sum_{(v_i,v_j)\in E(G)} \frac{1}{\sqrt{d_i\,d_j}}$$

and the two Zagreb indices [5, 6]

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

are the oldest and most thoroughly studied.

In the above formulas, as well as throughout the entire text, G denotes a graph whose vertex and edge sets are $V(G)$ and $E(G)$, respectively. An edge of G, connecting the vertices v_i nd v_j is denoted by (v_i, v_j). The number of vertices and edges of G is denoted by n and m, respectively, i. e., $|V(G)| = n$ and $|E(G)| = m$. The degree (= number of first neighbors) of the vertex v_i is denoted by d_i.

In 1972 the quantities $M_1 = M_1(G)$ and $M_2 = M_2(G)$ were found to occur within certain approximate expressions for the total π-electron energy [5]. In 1975 these graph invariants were proposed to be measures of branching of the carbon–atom skeleton [6]. The name "Zagreb index" (or, more precisely, "Zagreb group index") seems to be first used in the review article [7]. For details of the mathematical theory and chemical applications of the Zagreb indices see the surveys [8–11], the papers [12–16], and the references cited therein.

In spite of the fact that the two Zagreb indices were introduced simultaneously and examined almost always together, relations between them were not considered until quite recently. Based on his *AutoGraphiX* conjecture–generating computer system, Pierre Hansen arrived at the inequality

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

which he conjectured to hold for all connected graphs. Soon after the announcement of this conjecture it could be shown [17] that there exist graphs for which (1) does not hold, but that it holds for all molecular graphs, i. e., connected graphs in which no vertex has degree greater than 4.

Although the work [17] appeared to completely settle Hansen's conjecture, it was just the beginning of a long series of studies [18–35] in which the validity or non-validity of either (1) or some generalized version of (1) was considered for various classes of graphs. These studies are summarized in two recent surveys [36, 37].

Curiously, however, in spite of such an extensive research on inequality (1), little attention was paid on the equality case, i. e., on the characterization of graphs for which

$$\frac{M_1}{n} = \frac{M_2}{m} \tag{2}$$

holds. The aim of the present work is to shed some light on this latter problem.

In the current mathematico–chemical literature, the relation (1) is usually referred to as the *Zagreb indices inequality*. If the equality case is excluded, then we speak of the *strict Zagreb indices inequality*. In view of this, in what follows we call (2) the *Zagreb indices equality*.

2. Elementary results

The original formulation of Hansen's conjecture was the following [17].

Conjecture 1. For all simple connected graphs G, inequality (1) holds, and the bound is tight for complete graphs.

It is elementary to see that the bound is tight (i. e., that equality (2) holds) if G is a regular graph of any degree $r > 0$. In order to see this, recall that for regular graphs $M_1(G) = n\,r^2$ and $M_2(G) = m\,r^2$. Recall also that the complete graph K_n is the regular graph of degree $n-1$.

We say that a graph G is biregular if its vertex degrees assume exactly two distinct values, say d_a and d_b, ($d_a \neq d_b$). Let the number of vertices of degree d_a and d_b be a and b, respectively. By definition, $a > 0$, $b > 0$, and we may assume that $a \leq b$. Clearly, $a + b = n$ and $a\,d_a + b\,d_b = 2m$. We distinguish between two types of biregular graphs: Biregular graphs of *class 1* have the property that no two vertices of the same degree are adjacent. In biregular graphs of *class 2* at least one edge connects vertices of equal degree.

Biregular graphs of class 1 are necessarily bipartite. The complete bipartite graphs $K_{a,b}$ belong to class 1.

Theorem 2. The Zagreb indices equality holds for biregular graphs of class 1, whereas for biregular graphs of class 2 the strict Zagreb indices inequality applies.

Proof. In the notation specified above, $M_1(G) = a\,d_a^2 + b\,d_b^2$. A biregular graph of class 1 has $a\,d_a$ edges incident to a vertex of degree d_a , and $b\,d_b$ edges incident to a vertex of degree d_b . Therefore, $a\,d_a = b\,d_b$. Then,

$$M_1(G) = (a\,d_a)\,d_a + (b\,d_b)\,d_b = (b\,d_b)\,d_a + (a\,d_a)\,d_b = (a+b)\,d_a\,d_b$$

i. e.,

$$M_1(G) = n\,d_a\,d_b \ . \tag{3}$$

In biregular graphs of class 1, all edges connect a vertex of degree d_a with a vertex of degree d_b . Consequently,

$$M_2(G) = m\,d_a\,d_b \ . \tag{4}$$

Equality (2) immediately follows from (3) and (4). This proves the first part of Theorem 2.

Consider now a biregular graph in which x edges connect two vertices of degree d_a , y edges connect two vertices of degree d_b , and z edges connect a vertex of degree d_a with a vertex of degree d_b . Then

$$\begin{aligned} x+y+z &= m \\ 2x+z &= a\,d_a \qquad (5) \\ 2y+z &= b\,d_b \qquad (6) \\ M_2 &= x\,d_a^2 + y\,d_b^2 + z\,d_a\,d_b \ . \end{aligned}$$

Bearing these relations in mind, we have

$$m\,M_1 - n\,M_2 = (x+y+z)(a\,d_a^2 + b\,d_b^2) - (a+b)(x\,d_a^2 + y\,d_b^2 + z\,d_a\,d_b)$$

which, by using Eqs. (5) and (6), can be transformed into

$$m\,M_1 - n\,M_2 = -(d_a - d_b)^2\,(x\,b + y\,a) \ . \tag{7}$$

Since, $d_a \neq d_b$ and $a > 0$, $b > 0$, the right–hand side of Eq. (7) will be zero if and only if $x = y = 0$, i. e., if and only if the considered biregular graph is of class 1. Otherwise, the right–hand side of (7) is negative.

This completes the proof of Theorem 2. ■

Corollary 3. There is no benzenoid graph G for which the Zagreb indices equality holds.

Proof. Just note that benzenoid graphs are biregular, with $d_a = 2$, $d_b = 3$. Each benzenoid graph possesses an edge that connects vertices of degree 2. In fact, it possesses at least six such edges. ■

Let a , b , and c be three positive integers, $1 \leq a < b < c \leq n-1$. The graph G is said to be triregular if for $1, 2, \ldots, n$, either $d_i = a$ or $d_i = b$ or $d_i = c$, and there exists at least one vertex of degree a, at least one vertex of degree b, and at least one vertex of degree c. If so, then G is a triregular graph of degrees a, b, and c, or for brevity, an (a, b, c)-triregular graph. Similarly, as in the case of biregular graphs, we distinguish two types of triregular graphs: Triregular graphs of *class 1* have the property that no two vertices of the same degree are adjacent. In triregular graphs of *class 2* at least one edge connects vertices of equal degree.

Theorem 4. There is no connected (a, b, c)-triregular graph G of class 1 that satisfies the Zagreb indices equality. Moreover, every connected (a, b, c)-triregular graph G of class 1 satisfies the strict Zagreb indices inequality.

Proof. Let G be a triregular graph of class 1. Let u, v, and w denote, respectively, the number of edges connecting vertices of degree a and b, of degree a and c, and of degree b and c. Then,

$$\begin{aligned}
M_1(G) &= \frac{u+v}{a}\,a^2 + \frac{u+w}{b}\,b^2 + \frac{v+w}{c}\,c^2 \\
M_2(G) &= u\,a\,b + v\,a\,c + w\,b\,c \\
n &= \frac{u+v}{a} + \frac{u+w}{b} + \frac{v+w}{c} \\
m &= u+v+w\,.
\end{aligned}$$

From this follows

$$\frac{M_1(G)}{n} - \frac{M_2(G)}{m} = -\frac{a^2\,(b-c)^2\,u\,v + [b^2\,(a-c)^2\,u + (a-b)^2\,c^2\,v]w}{(u+v+w)[b\,c(u+v) + a\,c\,(u+w) + a\,b\,(v+w)]}\,.$$

Since $1 \leq a < b < c$, the expression $a^2\,(b-c)^2\,u\,v + [b^2\,(a-c)^2\,u + (a-b)^2\,c^2\,v]w$ equals zero if at least two out of the three parameters u, v, and w equal zero, i. e., G satisfies the equality only if G is disconnected. Otherwise, the above expression is negative, which implies that any connected triregular graph of class 1 satisfies the strict Zagreb indices inequality. ■

In Theorem 4, the requirement for connectedness is essential. As shown in the subsequent section, several graphs of the type $K_p \cup K_{a,b}$, which are disconnected and triregular of class 2, satisfy the Zagreb indices equality. Finding a connected example (if such does exist) remains a task for the future.

The subdivision graph $S(G)$ of a graph G is obtained by inserting a new vertex (of degree 2) on every edge of G.

Theorem 5. The Zagreb indices inequality is obeyed by the subdivision graph $S(G)$ of any graph G. The Zagreb indices equality holds if and only if the parent graph G is regular of degree $r > 0$.

Proof. If G is a regular graph of non-zero degree r, then $S(G)$ is biregular of class 1, and then by Theorem 2 the equality (2) holds for $S(G)$.

It remains to demonstrate that if G is not regular, then the strict Zagreb indices inequality holds.

If G has n vertices and m edges, then $S(G)$ has $n + m$ vertices and $2m$ edges. In addition, if the vertex degrees of G are $d_1, d_2, \ldots, d_n$, then the vertex degrees of $S(G)$ are $d_1, d_2, \ldots, d_n$ and 2 (m times). Therefore,

$$\begin{aligned} M_1(S(G)) &= M_1(G) + 4m \\ M_2(S(G)) &= \sum_{i=1}^{n} d_i \; (2 \cdot d_i) = 2\, M_1(G) \; . \end{aligned}$$

In the case of $S(G)$, inequality (1) will hold if

$$\frac{M_1(G) + 4m}{n + m} \leq \frac{2\, M_1(G)}{2m}$$

which is directly transformed into

$$M_1(G) \geq \frac{4m^2}{n} \; . \tag{8}$$

The variance of the vertex degrees of the graph G is

$$Var(d) = \frac{1}{n} \sum_{i=1}^{n} d_i^2 - \left(\frac{1}{n} \sum_{i=1}^{n} d_i \right)^2$$

i. e.,

$$Var(d) = \frac{M_1(G)}{n} - \left(\frac{2m}{n}\right)^2$$

which, in view of the fact that the variance cannot be negative–valued, leads to inequality (8). Consequently, inequality (1) holds for $S(G)$. If not all vertex degrees of G are equal, then their variance is greater than zero, implying that inequality (8), and therefore also inequality (1), are strict. ■

3. Simple examples for the validity of Zagreb indices equality

We start with a few "unsuccessful" examples, all pertaining to disconnected graphs. Let, as usual, K_n, C_n, and P_n denote, respectively, the n-vertex complete graph, cycle, and path. Let further $K_{a,b}$ be the complete bipartite graph on $a+b$ vertices.

Elementary calculation shows that

$$\begin{aligned} M_1(K_n) &= n(n-1)^2 &;\quad& M_2(K_n) = \frac{1}{2}\,n(n-1)^3 \\ M_1(C_n) &= 4n &;\quad& M_2(C_n) = 4n \\ M_1(P_n) &= 4(n-2)+2 &;\quad& M_2(P_n) = 4(n-3)+4 \quad \text{provided } n \geq 3 \\ M_1(K_{a,b}) &= ab(a+b) &;\quad& M_2(K_{a,b}) = a^2\,b^2\,. \end{aligned}$$

For $n=1$ and $n=2$ the Zagreb indices of the path are computed by using the fact that then $P_n \cong K_n$.

Example 6. Let $G \cong K_p \cup K_q$. Then the Zagreb indices inequality (1) holds for all $p,q \geq 1$, whereas the Zagreb indices equality (2) holds if and only if $p=q$. This latter case is trivial, because for $p=q$ the graph G is regular.

Proof. In this case $n=p+q$ and $m=\frac{1}{2}\,p(p-1)+\frac{1}{2}\,q(q-1)$, and then (1) becomes

$$\frac{p(p-1)^2+q(q-1)^2}{p+q} \leq \frac{\frac{1}{2}\,p(p-1)^3+\frac{1}{2}\,q(q-1)^3}{\frac{1}{2}\,p(p-1)+\frac{1}{2}\,q(q-1)}$$

which can be transformed into

$$(p-q)^2\,(p+q-2) \geq 0$$

from which the claim of Example 6 immediately follows. ■

Example 7. Let $G \cong K_p \cup C_q$. Then inequality (1) holds for all $p \geq 1$, $q \geq 3$, whereas Eq. (2) holds if and only if $p=3$, $q \geq 3$. This latter case is trivial, because for $p=3$ and $q \geq 3$ the graph G is regular (of degree 2).

Proof. This time inequality (1) reads:

$$\frac{p(p-1)^2+4q}{p+q} \leq \frac{\frac{1}{2}\,p(p-1)^3+4q}{\frac{1}{2}\,p(p-1)+q}$$

which for any positive value of q can be simplified as

$$(p-3)^2\,(p+1) \leq 0\ .$$

The claim of Example 7 follows. ■

Example 8. Let $G \cong K_p \cup P_q$, $q \geq 3$. Then the strict Zagreb indices inequality holds for all p, q .

Proof. This time inequality (1) reads:

$$\frac{p(p-1)^2+4q-6}{p+q} \leq \frac{\frac{1}{2}\,p(p-1)^3+4q-8}{\frac{1}{2}\,p(p-1)+q-1}$$

which after a lengthy calculation is reduced to

$$\frac{pq}{2}\,\left(p^3-5\,p^2+3p+9\right)+(p^3+p^2-10\,p-6)+2q \geq 0\ .$$

Now, the polynomials $p^3-5\,p^2+3p+9$ and $p^3+p^2-10\,p-6$ are equal to zero for $p=3$ and are greater than zero for $p>3$. This implies the claim of Example 7. ■

It can be easily checked that the strict Zagreb indices inequality holds also for $p \geq 1$, $q=2$ and $p \geq 2$, $q=1$, except for $p=q=2$, in which case $K_p \cup P_q$ is regular (and thus the Zagreb indices equality applies).

In a similar manner one can verify the following two examples:

Example 9. Let $G \cong C_p \cup P_q$. Then the strict Zagreb indices inequality (1) holds for all p, q .

Example 10. Let $G \cong P_p \cup P_q$. Then the Zagreb indices inequality (1) holds for all p, q , whereas the Zagreb indices equality (2) holds if and only if $p=q=2$ and $p=q=3$. These two cases are trivial, because for $p=q=2$, G is regular and for $q=p=3$, G is biregular of class 1.

Example 11. Let $G \cong C_p \cup K_{a,b}$, $a \leq b$. Then inequality (1) holds for all p, a, b , except for $p \geq 3$, $a=1$, $b \geq 5$. Equality (2) is satisfied only in the following two cases:

$p \geq 3$, $a = b = 2$ and $p \geq 3$, $a = 1$, $b = 4$. The first of these cases is trivial, because the G is regular (of degree 2).

Proof. This time inequality (1) reads:

$$\frac{4p + ab(a+b)}{p + (a+b)} \leq \frac{4p + a^2\, b^2}{p + ab}$$

which for any positive value of p is reduced to

$$(a + b - ab)(ab - 4) \leq 0 \; .$$

The claim of Example 11 is now obtained after an easy analysis. ■

We note here that the $K_3 \cup K_{1,5}$ is the simplest graph for which the Zagreb indices inequality is violated. Also, $K_3 \cup K_{1,4}$ is the simplest non-trivial example for the validity of the Zagreb indices equality. These observations were made already in the paper [17].

We conclude this section by two examples which provide a multitude of graphs satisfying the Zagreb indices equality.

Example 12. Let $G \cong K_p \cup K_{a,b}$, $a \leq b$. Then the Zagreb indices equality holds for a large number of below specified cases.

Proof. This time inequality (1) reads:

$$\frac{p(p-1)^2 + ab(a+b)}{p + (a+b)} \leq \frac{\frac{1}{2}\, p(p-1)^3 + a^2\, b^2}{\frac{1}{2}\, p(p-1) + ab}$$

which after a lengthy calculation is transformed into

$$\left[(p-1)^2 - ab\right] \left[(p-1)(a+b) - 2ab\right] \geq 0 \; .$$

Equality is attained if either

$$(p-1)^2 - ab = 0 \tag{9}$$

or

$$(p-1)(a+b) - 2ab = 0 \; . \tag{10}$$

The solutions of of Eq. (9) are easy and they come from the factorization of the type $a \times b$ of $(p-1)^2$. In particular, for any value of p , the graphs $K_p \cup K_{1,(p-1)^2}$ and $K_p \cup K_{p-1,p-1}$ satisfy Eq. (2). There, however, are other solutions, some of which are listed here:

$$p = 5\ ,\ \ a = 2\ ,\ \ b = 8$$

$$p = 7\ ,\ \ a = 2\ ,\ \ b = 18$$

$$p = 7\ ,\ \ a = 3\ ,\ \ b = 12$$

$$p = 7\ ,\ \ a = 4\ ,\ \ b = 9$$

$$p = 9\ ,\ \ a = 2\ ,\ \ b = 32$$

$$p = 9\ ,\ \ a = 4\ ,\ \ b = 16$$

$$p = 10\ ,\ \ a = 3\ ,\ \ b = 27 \qquad \text{etc.}$$

Among the solutions of Eq. (10) we first find those for which $a = b$. These read: $K_p \cup K_{p-1,p-1}$. However, there exist other solutions. Namely, Eq. (10) is equivalent to

$$(p-1)^2 = (2a-p+1)(2b-p+1)$$

or

$$(p-1)^2 = p_1 \times p_2$$

where $p_1 = 2a - p + 1$ and $p_2 = 2b - p + 1$.

Exactly, all integer solutions of (10) come from the factorization of the type $p_1 \times p_2$ of $(p-1)^2$ when $p_1 + p - 1$ and $p_2 + p - 1$ are even. Then, the integer solutions of Eq. (10) are the triples of integers $[(p_1 + p - 1)/2\,,\ (p_2 + p - 1)/2\,,\ p]$. Some of these solutions (for $a \neq b$) are listed here:

$$p = 4\ ,\ \ a = 2\ ,\ \ b = 6$$

$$p = 6\ ,\ \ a = 3\ ,\ \ b = 15$$

$$p = 7\ ,\ \ a = 4\ ,\ \ b = 12$$

$$p = 8\ ,\ \ a = 4\ ,\ \ b = 28$$

$$p = 9\ ,\ \ a = 5\ ,\ \ b = 20$$

$$p = 9\ ,\ \ a = 6\ ,\ \ b = 12$$

$$p = 10\ ,\ \ a = 5\ ,\ \ b = 45$$

$$p = 10\ ,\ \ a = 6\ ,\ \ b = 18 \qquad \text{etc.}$$

Example 13. Let $G \cong K_{a,b} \cup K_{c,d}$, $a \leq b$, $c \leq d$. Then the Zagreb indices equality holds for a large number of below specified cases.

Proof. This time inequality (1) reads:

$$\frac{ab(a+b)+cd(c+d)}{(a+b)+(c+d)} \leq \frac{a^2\,b^2+c^2\,d^2}{ab+cd}$$

which can be reduced to

$$(ab-cd)\,[ab(c+d)-cd(a+b)] \geq 0 \; .$$

Equality is attained if either

$$ab = cd \tag{11}$$

or

$$ab(c+d) = cd(a+b) \; . \tag{12}$$

Eq. (11) has infinitely many solutions, whose characterization is easy. Some of these are:

$$a=6 \; , \; b=12 \; , \; c=5 \; , \; d=20$$
$$a=9 \; , \; b=18 \; , \; c=8 \; , \; d=24$$
$$a=16 \; , \; b=48 \; , \; c=15 \; , \; d=60 \qquad \text{etc.}$$

The solutions of (12) are less easy to characterize, and this remains a task for the future. We found infinite quadruplets of integers a, b, c, d for which $K_{a,b} \cup K_{c,d}$ satisfies Eq. (2). One of these is:

$$a = y(xz+1) \; , \; b = xyz(xz+1) \; , c = x(yz+1) \; , \; d = xyz(yz+1)$$

where x, y, z are arbitrary positive integers.

Remark 14. In the case of graphs considered in Example 13, the Zagreb indices inequality is violated for infinitely many quartets of numbers (a, b, c, d) . For instance, if $a = 3$, then (1) is violated by $K_{a,b} \cup K_{c,d}$ for:

$$a=3 \; , \; b=7 \; , \; c=4 \; , \; d=5$$
$$a=3 \; , \; b=8 \; , \; c=4 \; , \; d=5$$
$$a=3 \; , \; b=9 \; , \; c=4 \; , \; d=6$$
$$a=3 \; , \; b=9 \; , \; c=5 \; , \; d=5$$
$$a=3 \; , \; b=10 \; , \; c=4 \; , \; d=6$$
$$a=3 \; , \; b=10 \; , \; c=4 \; , \; d=7$$
$$a=3 \; , \; b=10 \; , \; c=5 \; , \; d=5 \; .$$

4. A connected example

Theorem 15. Let G be a simple connected graph with maximal degree at most 4. Then the Zagreb indices equality (2) holds if and only if G is regular or G is biregular of class 1. On the other hand, there exist connected graphs of maximal degree 5 that are neither regular, nor bipartite, which satisfy Eq. (2).

Proof. In a similar way as in the paper [17], it can be shown that Eq. (2) holds if and only if:

$$\sum \left[\left(i^2j^2\ell + i^2j^2k + k^2\ell^2j + k^2\ell^2i - i^2jk\ell - ij^2k\ell - ijk^2\ell - ijk\ell^2 \right) \cdot \frac{m_{ij} \cdot m_{k\ell}}{i \cdot j \cdot k \cdot \ell} \right] = 0$$

where the summation goes over all integers i, j, k, ℓ, such that $i \leq j$ and $k \leq \ell$, and where m_{ij} denotes the number of edges connecting a vertex of degree i with a vertex of degree j. Similarly, as in [17], let us denote

$$i^2j^2\ell + i^2j^2k + k^2\ell^2j + k^2\ell^2i - i^2jk\ell - ij^2k\ell - ijk^2\ell - ijk\ell^2$$

by $g(i, j, k, \ell)$. The values of $g(i, j, k, \ell)$ where $1 \leq i, j, k, \ell \leq 4$ are presented by the following table [17]:

		$\{i,j\}$									
		$\{1,1\}$	$\{1,2\}$	$\{1,3\}$	$\{1,4\}$	$\{2,2\}$	$\{2,3\}$	$\{2,4\}$	$\{3,3\}$	$\{3,4\}$	$\{4,4\}$
$\{k,\ell\}$	$\{1,1\}$	0	1	4	9	12	35	70	96	187	360
	$\{1,2\}$	1	0	1	4	8	32	72	105	220	448
	$\{1,3\}$	4	1	0	1	4	27	70	108	243	520
	$\{1,4\}$	9	4	1	0	0	20	64	105	256	576
	$\{2,2\}$	12	8	4	0	0	8	32	60	160	384
	$\{2,3\}$	35	32	27	20	8	0	8	27	108	320
	$\{2,4\}$	70	72	70	64	32	8	0	6	64	256
	$\{3,3\}$	96	105	108	105	60	27	6	0	27	168
	$\{3,4\}$	187	220	243	256	160	108	64	27	0	64
	$\{4,4\}$	360	448	520	576	384	320	256	168	64	0

Table 1. Values of the function $g(i, j, k, \ell)$.

From Table 1 it can be easily seen that either all edges must be of the same type (i. e., for some fixed values of i and j, all edges connect a vertex of degree i with a vertex of degree j) or there are only edges of types {1,4} and {2,2}. However, the latter case is not possible since then the graph would not be connected.

On the other hand, this does not have to hold for the graphs of maximal degree 5. Let us consider a family of graphs $G_{x,y,z}$, $x, y, z \geq 1$, defined in the following way:

We start with the graph $H_{x,y}$ consisting of x copies of $K_{3,3}$ and y copies of $K_{2,5}$. Denote the vertices of the i-th copy of $K_{3,3}$ in such way that vertices $p_{i,1}, p_{i,2}$, and $p_{i,3}$ are in one class and $q_{i,1}, q_{i,2}$, and $q_{i,3}$ are in the other class. Similarly, denote the vertices of the i-th copy of $K_{2,5}$ in such a way that $u_{i,1}$ and $u_{i,2}$ belong to one class and $v_{i,1}, \ldots, v_{i,5}$ to the other class. Then we define

$$\begin{aligned} G_{x,y} &= H_{x,y} \\ &- \left\{ \begin{array}{l} p_{1,3}\,q_{1,3}\,,\ p_{2,1}\,q_{2,1}\,,\ p_{2,3}\,q_{2,3}\,,\ p_{3,1}\,q_{3,1}\,,\ p_{3,3}\,q_{3,3}\,,\ldots\,,\ p_{x,1}\,q_{x,1}\,,\ p_{x,3}\,q_{x,3}\,, \\ u_{1,1}\,v_{1,1}\,,\ u_{1,2}\,v_{1,5}\,,\ u_{2,1}\,v_{2,1}\,,\ u_{2,2}\,v_{2,5}\,,\ldots\,,\ u_{y-1,1}\,v_{y-1,1}\,,\ u_{y-1,2}\,v_{y-1,5}\,,\ u_{y,1}\,v_{y,1} \end{array} \right\} \\ &+ \left\{ \begin{array}{l} p_{1,3}\,q_{2,1}\,,\ q_{1,3}\,p_{2,1}\,,\ldots\,,\ p_{x-1,3}\,q_{x,1}\,,\ q_{x-1,3}\,p_{x,1}\,,\ p_{x,3}\,u_{1,1}\,,\ q_{x,3}\,v_{1,1}\,, \\ u_{1,2}\,v_{2,1}\,,\ v_{1,5}\,u_{2,1}\,,\ldots\,,\ u_{y-1,2}\,v_{y,1}\,,\ v_{y-1,5}\,u_{y,1} \end{array} \right\}. \end{aligned}$$

Finally, the graph $G_{x,y,z}$ is obtained by replacing the edge $u_{y,2}\,v_{y,5}$ by a path of length $z+1$.

We illustrate this construction by the graph $G_{3,2,1}$ depicted in Figure 1.

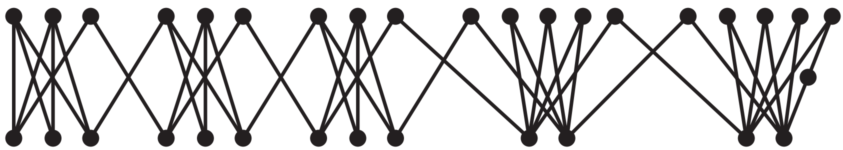

Figure 1. The graph $G_{3,2,1}$.

Note that:

$$\begin{aligned} M_2(G_{x,y,z}) &= 9 \cdot 9 \cdot x + 10 \cdot 10 \cdot y + 6 + 15 - 9 - 10 + 4z \\ m(G_{x,y,z}) &= 9x + 10y + z \\ M_1(G_{x,y,z}) &= 6 \cdot 9 \cdot x + 5 \cdot 4 \cdot y + 2 \cdot 25 \cdot y + 4z \\ n(G_{x,y,z}) &= 6 \cdot x + 7 \cdot y + z\,. \end{aligned}$$

Simple calculation shows that $M_1(G_{x,y,z})/n(G_{x,y,z}) = M_2(G_{x,y,z})/m(G_{x,y,z})$ if and only if

$$z = \frac{-12x - 14y + 3xy}{2 + 15x + 18y}\,.$$

One such combination is $(x,y,z)=(14,38,1)$. Hence,

$$\frac{M_1(G_{14,38,1})}{n}=\frac{M_2(G_{14,38,1})}{m}\ .$$

■

Remark 16. One can show that there are infinitely many graphs $G_{x,y,z}$ satisfying the Zagreb indices equality. Observe the family of graphs $H_u = G_{6+12u,18+82u+90u^2,2u}$. For it,

$$\begin{aligned} M_2(H_u) &= 2288 + 9180\,u + 9000\,u^2 \\ m(H_u) &= 234 + 930\,u + 900\,u^2 \\ M_1(H_u) &= 1584 + 6396\,u + 6300\,u^2 \\ n(H_u) &= 162 + 648\,u + 630\,u^2\ . \end{aligned}$$

The fact that equality (2) holds for H_u can now be verified by simple calculation.

5. A general construction method

We start first with a trivial example. Suppose that there is an (n,m)-graph G satisfying the relation

$$\frac{M_1(G)}{n}\ \rho\ \frac{M_2(G)}{m} \tag{13}$$

where ρ is one of the symbols $<$, $=$, or $>$.

Let $G_2 = G' \cup G''$ be the graph consisting of two disjoint components G', G'', each being isomorphic to G. Then, evidently,

$$n(G_2)=2n\ \ ;\ \ m(G_2)=2m\ \ ;\ \ M_1(G_2)=2\,M_1(G)\ \ ;\ \ M_2(G_2)=2\,M_2(G)$$

and therefore

$$\frac{M_1(G_2)}{n(G_2)}\ \rho\ \frac{M_2(G_2)}{m(G_2)}$$

is satisfied.

Let e'_{rs} be any edge of the graph G'. Let this edge connect the vertices v'_r and v'_s.

Let G'' be a graph isomorphic to G', and let its edge and vertices corresponding to e'_{rs}, v'_r, and v'_s, be denoted by e''_{rs}, v''_r, and v''_s, respectively.

Construct the graph G'_2 in the following way.

Start with $G_2 = G' \cup G''$. Delete from it the edges e'_{rs} and e''_{rs}, and insert new edges between the vertices v'_r, and v''_s, and between v''_r, and v'_s.

By the transformation $G_2 \to G_2'$, the number of vertices and edges remains the same, as well as the degrees of the vertices v_r', v_s', v_r'', and v_s''. It is elementary to verify that also the two Zagreb indices remain unchanged. This immediately leads to the following:

Theorem 17. If G is a graph satisfying the relation (13), then also the above described graph G_2' satisfies this relation.

From Theorem 15 and the examples constructed in its proof we know that there exist connected graphs (which are not trees), satisfying the Zagreb indices equality.

Corollary 18. If G is a connected graph satisfying the Zagreb indices equality, and if its edge e_{rs} belongs to a cycle, then also the above described graph G_2' is connected and satisfies the Zagreb indices equality.

Since the graph G_2' in Corollary 18 also contains an edge belonging to a cycle, the construction of connected graphs satisfying the Zagreb indices equality can be continued as libitum.

6. Union of graphs and the Zagreb indices inequality

As before, the union $G_1 \cup G_2$ of an (n_1, m_1)-graph G_1 and an (n_2, m_2)-graph G_2 with disjoint vertex sets V_1 and V_2 and edge sets E_1 and E_2 is the $(n_1 + n_2, m_1 + m_2)$-graph with vertex set $V_1 \cup V_2$ and edge set $E_1 \cup E_2$.

Suppose that the graphs G_1 and G_2 satisfy the Zagreb indices inequalities

$$\frac{M_1(G_1)}{n_1} \leq \frac{M_2(G_1)}{m_1} \qquad \text{and} \qquad \frac{M_1(G_2)}{n_2} \leq \frac{M_2(G_2)}{m_2} \,.$$

If also their union satisfies the Zagreb indices inequality, i. e.,

$$\frac{M_1(G_1 \cup G_2)}{n_1 + n_2} \leq \frac{M_2(G_1 \cup G_2)}{m_1 + m_2}$$

then we say that G_1 and G_2 satisfy the *Zagreb indices transitivity relation* $\mathcal{T} = \mathcal{T}(G_1, G_2)$.

Not all graphs obey the relation $\mathcal{T}$. An earlier encountered example for the violation of $\mathcal{T}$ is $C_3 \cup K_{1,5}$.

In what follows, we investigate when the union of $G = G_1 \cup G_2$ also satisfies the Zagreb indices inequality, or equivalently when

$$\frac{M_1(G)}{M_2(G)} = \frac{M_1(G_1 \cup G_2)}{M_2(G_1 \cup G_2)} \leq \frac{n}{m} \tag{14}$$

is true, where $n = n_1 + n_2$ and $m = m_1 + m_2$. Obviously,

$$\frac{M_1(G_1 \cup G_2)}{M_2(G_1 \cup G_2)} = \frac{M_1(G_1) + M_1(G_2)}{M_2(G_1) + M_2(G_2)} . \tag{15}$$

Let $M_2(G_1) = u_1\, m_1$ and $M_2(G_2) = u_2\, m_2$. Since for every graph H it is true that $M_2(H) \geq |E(H)|$, it follows that $u_1 \geq 1$ and $u_2 \geq 1$. Thus, from (15) we obtain

$$\frac{M_1(G)}{M_2(G)} = \frac{M_1(G_1) + M_1(G_2)}{u_1\, m_1 + u_2\, m_2} \leq \frac{u_1\, n_1 + u_2\, n_2}{u_1\, m_1 + u_2\, m_2} . \tag{16}$$

Notice that if G_1 and G_2 satisfy the Zagreb indices equality, then in (16) the last relation is also equation. If $u_1 = u_2$, then the inequality (14) is satisfied, and we immediately have the following result.

Theorem 19. Let G_1 be an (n_1, m_1)-graph and let G_2 be an (n_2, m_2)-graph, both satisfying the Zagreb indices inequality. If $M_2(G_1)/m_1 = M_2(G_2)/m_2$, then $\mathcal{T}(G_1, G_2)$ holds.

Trivial cases that satisfy the requirements of Theorem 19 are found in the Examples in Section 3.

From (16) we immediately have the following result.

Theorem 20. Let G_1 be an (n_1, m_1)-graph and let G_2 be an (n_2, m_2)-graph, both satisfying the Zagreb indices inequality. Then $\mathcal{T}(G_1, G_2)$ holds if

(a) $n_1 = n_2$ and $m_1 = m_2$, or

(b) $n_1 = m_1$ and $n_2 = m_2$.

Under the same conditions, if the Zagreb indices equality holds for G_1 and G_2 , then it also holds for $G_1 \cup G_2$.

Examples satisfying condition (a) are when G_1 and G_2 are trees on same number of vertices, or when G_1 and G_2 are isomorphic. An example that satisfies (b) is when G_1 and G_2 are unicyclic graphs.

Now we assume that $u_2 > u_1$. (Since the graph union is a commutative operation, the same analysis applies for the case $u_2 < u_1$.) Let $u = u_2/u_1$. Then from (16),

$$\frac{M_1(G_1 \cup G_2)}{M_2(G_1 \cup G_2)} \leq \frac{n_1 + u\, n_2}{m_1 + u\, m_2} .$$

For $u > 1$, the inequality $\dfrac{n_1 + u\, n_2}{m_1 + u\, m_2} \leq \dfrac{n_1 + n_2}{m_1 + m_2}$ is satisfied when $\dfrac{n_2}{m_2} \leq \dfrac{n_1}{m_1}$.

Theorem 21. Let G_1 be an (n_1, m_1)-graph and let G_2 be an (n_2, m_2)-graph, both satisfying the strict Zagreb indices inequality (resp. the Zagreb indices equality). If

$M_2(G_1)/m_1 < M_2(G_2)/m_2$, then their union satisfies the strict Zagreb indices inequality (resp. the Zagreb indices equality) if $n_2/m_2 < n_1/m_1$ (resp. $n_2/m_2 = n_1/m_1$).

We would like to stress that the condition $n_2/m_2 < n_1/m_2$ (resp. $n_2/m_2 = n_1/m_2$) from Theorem 21 is sufficient, but not necessary. There are graphs G_1 and G_2 with $M_2(G_1)/m_1 < M_2(G_2)/m_2$ and $n_2/n_1 > m_2/m_1$ that satisfy the Zagreb indices inequality. For example, consider the case when G_1 is P_n and G_2 is S_q, for $n \geq q \geq 3$. The reason is that in those cases we have the strict inequality $M_1(G_1 \cup G_2)/M_2(G_1 \cup G_2) < (n_1 + u\,n_2)/(m_1 + u\,m_2)$, and $(n_1 + u\,n_2)/(m_1 + u\,m_2) \geq (n_1 + n_2)(m_1 + m_2)$ does not necessarily imply $M_1(G_1 \cup G_2)/M_2(G_1 \cup G_2) > (n_1 + n_2)(m_1 + m_2)$.

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