Graph Classes (Dis)satisfying the Zagreb Indices Inequality

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Some classes of graphs (dis)satisfying the Zagreb indices inequality*

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Abstract

Recently Hansen and Vukičević [10] proved that the inequality $M_1/n \leq M_2/m$, where M_1 and M_2 are the first and second Zagreb indices, holds for chemical graphs, and Vukičević and Graovac [17] proved that this also holds for trees. In both works is given a distinct counterexample for which this inequality is false in general. Here, we present some classes of graphs with prescribed degrees, that satisfy $M_1/n \leq M_2/m$. Namely every graph G whose degrees of vertices are in the interval $[c, c + \lceil\sqrt{c}\,\rceil]$ for some integer c, satisfies this inequality. In addition, we prove that for any $\Delta \geq 5$, there is an infinite family of graphs of maximum degree Δ such that the inequality is false. Moreover, an alternative and slightly shorter proof for trees is presented, as well as for unicyclic graphs.

Keywords: First Zagreb index, second Zagreb index

1 Introduction

The first and second Zagreb indices are among the oldest topological indices [2, 7, 9, 12, 15], defined in 1972 by Gutman [8], and are given different names in the literature, such as the Zagreb group indices, the Zagreb group parameters and most often, the Zagreb indices. Zagreb indices were among the first indices introduced, and have since been used to study molecular complexity, chirality, ZE-isomerism and hetero-systems. Overall, Zagreb indices exhibited a potential applicability for deriving multi-linear regression models.

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In what follows, let $G = (V, E)$ be a simple graph with $n = |V|$ vertices and $m = |E|$ edges. These indices are defined as

$$M_1(G) = \sum_{v \in V} d(v)^2 \quad \text{and} \quad M_2(G) = \sum_{uv \in E} d(u)d(v).$$

For the sake of simplicity, we will often use M_1 and M_2 instead of $M_1(G)$ and $M_2(G)$, respectively. The article [14] was responsible for new research wave concerning Zagreb indices. See [5, 6, 13, 11, 20, 21, 22] for more work done on these indices. Comparing the values of these indices on the same graph gives interesting results. At first the next conjecture was proposed [1, 3, 4]:

Conjecture 1.1. *For all simple graphs G,*

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

and the bound is tight for complete graphs.

If the graph is regular then this bound is tight, but it is also tight if G is a star. This inequality holds for trees [17], graphs of maximum degree four, so called chemical graphs [10] and unicyclic graphs [19], but this inequality does not hold in general. Hansen and Vukičević [10], and Vukičević and Graovac [17], gave examples of graphs dissatisfying the inequality (1).

As we said before, there are infinitely many graphs that satisfy $M_1/n \leq M_2/m$: regular graphs, stars, trees and unicyclic graphs. Here we present some other classes of graphs with prescribed degrees for which (1) holds: graphs with only two types of vertex degrees and graphs with vertex degrees in any interval of length three. We came to the conclusion that there are arbitrary long intervals of vertex degrees for a graph G such that G satisfies the inequality (1). Namely, every graph G such that its vertices degrees are in the interval $[c, c + \lceil\sqrt{c}\,\rceil]$ for any integer c, satisfies this inequality. Also we prove that for any $\Delta \geq 5$, there is an infinite family of graphs of maximum degree Δ such that the inequality is false. An alternative and slightly shorter proof for trees is presented, as well as for unicyclic graphs.

Denoted by $K_{a,b}$ the *complete bipartite* graph with a vertices in one class and b vertices in the other class. A star with k edges is called a *k-star,* we denote it by S_k. Denote by P_k a path of length k, where k is the number of vertices/edges, it is also called a *k-path.* Since, we will discuss conditions when the inequality (1) holds, for the sake of simplicity, we will introduce $m_{i,j}$ to be the number of edges that connect vertices of degrees i and j in the graph G. Then as shown in [10]:

$$\frac{M_2}{m} - \frac{M_1}{n} = \sum_{\substack{i \leq j, k \leq l \\ (i,j),(k,l) \in \mathbb{N}^2}} \left[\left(i\,j \left(\frac{1}{k} + \frac{1}{l} \right) + k\,l \left(\frac{1}{i} + \frac{1}{j} \right) - i - j - k - l \right) m_{i,j}\, m_{k,l} \right]. \tag{2}$$

2 Short good intervals

It is easy to see that if G is a k-regular graph, then (1) is valid, since

$$\frac{M_1}{n} = k^2 = \frac{M_2}{m}.$$

As Conjecture 1.1 is false in general, but true for k-regular graphs, one may wander if it also holds for "almost regular" graphs, i.e. graphs with only few vertex degrees. Now, we verify that this holds for graphs with only two vertex degrees.

Proposition 2.1. *Let $x, y \in \mathbb{N}$, and let G be a graph with n vertices, m edges, and $d(v) \in \{x, y\}$ for every vertex v of G. Then, the inequality (1) holds for G.*

Proof. Since $d(v) = x$ or y for every vertex $v \in V$, we conclude $m_{i,j} = 0$, whenever $i, j \notin \{x, y\}$. By (2), we infer

$$\begin{aligned} \frac{M_2}{m} - \frac{M_1}{n} &= 2\left[\frac{x^3(x-y)^2}{x^3y} m_{x,x} m_{x,y} + \frac{2xy(x-y)^2(x+y)}{x^2y^2} m_{x,x} m_{y,y} + \frac{y^3(x-y)^2}{xy^3} m_{x,y} m_{y,y}\right] \\ &= 2(x-y)^2\left[\frac{1}{y} m_{x,x} m_{x,y} + 2\left(\frac{1}{x} + \frac{1}{y}\right) m_{x,x} m_{y,y} + \frac{1}{x} m_{x,y} m_{y,y}\right] \\ &\geq 0. \end{aligned}$$

□

Let $D(G)$ be the set of the vertex degrees of G, i.e. $D(G) = \{d(v) \,|\, v \in V\}$. Motivated by the above proposition, one may be interested to look for sets D with property that for every graph G with $D(G) \subseteq D$ the inequality (1) holds. So it is reasonable to introduce the following definition: A set S of integers is *good* if for every graph G with $D(G) \subseteq S$, the inequality (1) holds. Otherwise, S is a *bad* set. Thus, by above any set of integers of size ≤ 2 is good.

Sometimes in order to examine whether the inequality (1) holds, one can consider whether $M_2/m - M_1/n$ is non-negative. The difference that we are considering is given by (2). For simplifying (2), we will define a function f, and study some of its properties. Now, for integers i, j, k, l, let

$$f(i, j, k, l) = i\,j\left(\frac{1}{k} + \frac{1}{l}\right) + k\,l\left(\frac{1}{i} + \frac{1}{j}\right) - i - j - k - l.$$

Then (2) can be restated simply as

$$\frac{M_2}{m} - \frac{M_1}{n} = \sum_{\substack{i \leq j, k \leq l \\ (i,j),(k,l) \in \mathbb{N}^2}} f(i, j, k, l) m_{i,j}\, m_{k,l}. \tag{3}$$

In the sequel, we study some properties of the function f.

Lemma 2.1. *The function f can be decomposed as*

$$f(i, j, k, l) = (ij - kl)\left(\frac{1}{k} + \frac{1}{l} - \frac{1}{i} - \frac{1}{j}\right).$$

Proof. Here we derive it

$$\begin{aligned} f(i, j, k, l) &= \frac{ij}{kl}(k + l) - (k + l) + \frac{kl}{ij}(i + j) - (i + j) \\ &= (k + l)\left[\frac{ij - kl}{kl}\right] + (i + j)\left[\frac{kl - ij}{ij}\right] \\ &= (ij - kl)\left(\frac{1}{k} + \frac{1}{l} - \frac{1}{i} - \frac{1}{j}\right). \end{aligned}$$

□

Now, the next lemma follows immediately by the above one.

Lemma 2.2. *For any integers i, j, k, l, it holds $f(i,j,k,l) < 0$ if and only if*

(a) $ij > kl$ *and* $\frac{1}{k} + \frac{1}{l} < \frac{1}{i} + \frac{1}{j}$, *or*

(b) $ij < kl$ *and* $\frac{1}{k} + \frac{1}{l} > \frac{1}{i} + \frac{1}{j}$.

Notice that the function f has some symmetry properties, namely for every i, j, k and l:

$$f(i,j,k,l) = f(j,i,k,l) \qquad \text{and} \qquad f(i,j,k,l) = f(k,l,i,j).$$

Determining the sign of the function f will help us to see whether the difference $M_2/m - M_1/n$ is non-negative. The following lemma gives us orderings of the integers i, j, k, and l, for which $f(i,j,k,l)$ can be negative.

Lemma 2.3. *If $f(i,j,k,l) < 0$ for some integers $i \leq j$ and $k \leq l$, then*

$$i < k \leq l < j \qquad \text{or} \qquad k < i \leq j < l.$$

Proof. Suppose first that $i \leq k$. There are only three possibilities:

- $i \leq j \leq k \leq l$;
- $i \leq k \leq j \leq l$;
- $i \leq k \leq l \leq j$.

If $i \leq j \leq k \leq l$, then $ij \leq kl$, but $\frac{1}{k} + \frac{1}{l} < \frac{1}{i} + \frac{1}{j}$, so this is impossible by Lemma 2.2(a). If $i \leq k \leq j \leq l$, then $ij \leq kl$ and $\frac{1}{k} + \frac{1}{l} < \frac{1}{i} + \frac{1}{j}$. This ordering is also impossible by Lemma 2.2(a). So, only possible ordering for $f(i,j,k,l)$ to be negative is $i \leq k \leq l \leq j$.

Now, if $i = k$ ($i = k \leq l \leq j$), then $ij \geq kl$ and $\frac{1}{i} + \frac{1}{j} > \frac{1}{k} + \frac{1}{l}$, which contradicts Lemma 2.2 (a). So, we conclude $i < k$. Similarly, one can show that $l \neq j$. Thus, we obtain the first ordering $i < k \leq l < j$ given in the lemma.

Suppose now $k \leq i$. Applying a similar argument as above, one obtains that $k < i \leq j < l$ is the only possible ordering. □

In Proposition 2.1 we have shown that for a graph G with $|D(G)| = 2$, the inequality (1) holds. Now, more general statement is presented.

Proposition 2.2. *Let $s, x \in \mathbb{N}$. For every graph G with n vertices, m edges and $D(G) \subseteq \{x - s, x, x + s\}$, the inequality (1) holds.*

Proof. The inequality (1) holds if $M_2/m - M_1/n$ is non-negative. The difference (3) is non-negative if for any integers i, j, k, l, the function $f(i,j,k,l)$ is non-negative. So we are interested whether $f(i,j,k,l)$ can be negative for some integers i, j, k, l. By Lemma 2.3, we may assume, up to symmetry, that the ordering of i, j, k, l is $i < k \leq l < j$. Since $i,j,k,l \in \{x-s, x, x+s\}$, we have that $f(i,j,k,l)$ can be negative only if $i = x - s, k = l = x$

and $j = x+s$. But $f(x-s, x+s, x, x) = \dfrac{1}{x-s} - \dfrac{2}{x} + \dfrac{1}{x+s} > 0$. Hence, we conclude that $\dfrac{M_2}{m} - \dfrac{M_1}{n} = \sum\limits_{\substack{i\le j, k\le l\\ (i,j),(k,l)\in\mathbb{N}^2}} f(i,j,k,l)\, m_{i,j}\, m_{k,l} > 0.$ □

By the previous proposition the following holds:

Corollary 2.1. *Any interval of length three is good.*

Notice that above result cannot be extended to any interval of length 4. For an example consider the graph $G(l,k,s)$ with $l = 4$ from Figure 2. It is obvious that $D\left(G(4,k,s)\right)$ is a subset of the interval $[2,5]$, but this graph for proper values of k and s does not satisfy the inequality (1), see Theorem 4.1.

The proof of Proposition 2.2 was motivation for more general conclusion.

Proposition 2.3. *The set of integers $\{a,b,c\}$, where $a < b < c$, is good if and only if*

(*a*) $b^2 \ge ac$ *and* $b(a+c) \ge 2ac$, *or*

(*b*) $b^2 \le ac$ *and* $b(a+c) \le 2ac$.

Proof. Since $a < b < c$, by Lemma 2.3 the function f can be negative in $f(i,j,k,l)$ only if either $i = a$, $k = l = b$ and $j = c$, or $k = a$, $i = j = b$ and $l = c$, i.e only $f(a,c,b,b) = f(b,b,a,c) = (ac-b^2)\left(\dfrac{2}{b} - \dfrac{1}{a} - \dfrac{1}{c}\right)$ can be negative. If (a) or (b) holds, then it is obvious that $f(i,j,k,l) \ge 0$ for any integers $i,j,k,l \in \{a,b,c\}$, and the inequality (1) is valid for every graph G such that $D(G) = \{a,b,c\}$.

For the other direction, suppose that neither (a) nor (b) holds. If this is the case, then only $f(a,c,b,b) < 0$. We construct a graph $G_{x,y}$, with $D(G_{x,y}) = \{a,b,c\}$, $m_{a,a} = m_{c,c} = 0$ and $m_{a,b} = m_{b,c} = 1$ (see Figure 1). The graph $G_{x,y}$ can be created in the following way:

- Make a sequence of x copies of $K_{a,c}$ and then continue that sequence with y copies of $K_{b,b}$.
- Chose an edge from the first $K_{a,c}$ graph an another edge from the second $K_{a,c}$. Then replace these edges by edges connecting the "a"-vertex from the first graph with "c"-vertex from the second graph, and another edge connecting the "c"-vertex from the first graph with "a"-vertex from the second graph. This way the degrees of the vertices are not changed. Continue this procedure between all x copies of $K_{a,c}$.
- Next, chose an edge from the last $K_{a,c}$ in the sequence and one edge from the first $K_{b,b}$ graph, replace these edges by edges connecting the "a"-vertex with one of the "b" vertices and the "c"-vertex with the other "b" vertex.
- The same procedure is applied between all consecutive graphs $K_{b,b}$ in the sequence and this way is $G_{x,y}$ constructed.

We emphasize that this binding procedure is done only once between $K_{a,c}$ and $K_{b,b}$ graphs.

Now,

$$\begin{aligned}\frac{M_2}{m}-\frac{M_1}{n} &= \sum_{\substack{i\le j,k\le l\\ i,j,k,l\in\{a,b,c\}}} f(i,j,k,l)m_{i,j}\,m_{k,l}\\ &= 2\left[f(a,c,b,b)m_{a,c}m_{b,b}+\big[f(a,c,a,b)+f(a,c,b,c)\big]m_{a,c}\right.\\ &\quad\left.+\big[f(a,b,b,b)+f(c,b,b,b)\big]m_{b,b}+f(a,b,b,c)\right].\end{aligned}$$

If we increase the number of $K_{a,c}$ and $K_{b,b}$ graphs, i.e. x and y, in the graph $G_{x,y}$, shown on Figure 1, then $m_{a,c}$ and $m_{b,b}$ will increase as well. For $m_{a,c}$ and $m_{b,b}$ big enough, the difference $M_2/m - M_1/n$ will be negative.

□

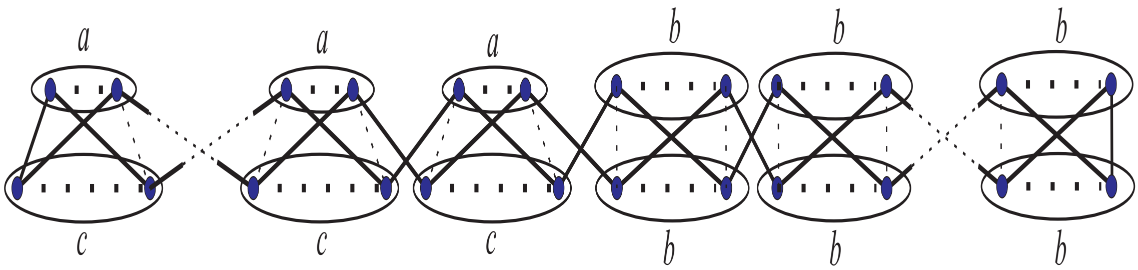

Figure 1: A connected graph G with $D(G)=\{a,b,c\}$. The edges that should be removed are drown with dashed lines.

3 Long good intervals

Our next goal is to determine long good intervals.

Lemma 3.1. *For integers c, i, j, and $p\le\lceil\sqrt{c}\,\rceil$ holds:*

$$c(c+p)>(c+i)(c+j)\quad\textit{if and only if}\quad i+j<p.$$

Proof. First notice that $ij\le\dfrac{(i+j)^2}{4}$. If $c(c+p)>(c+i)(c+j)$ and $i+j\ge p$, then

$$\begin{aligned}c^2+cp &> c^2+(i+j)c+ij\\ cp &> (i+j)c+ij,\end{aligned}$$

which is impossible. For the other direction, suppose that $i+j<p$. Then

$$\begin{aligned}(c+i)(c+j) &= c^2+(i+j)c+ij\\ &\le c^2+c(i+j)+\frac{(i+j)^2}{4}\\ &\le c^2+c(p-1)+\frac{(p-1)^2}{4}\\ &< c(c+p)-c+\frac{(\sqrt{c})^2}{4}\\ &< c(c+p).\end{aligned}$$

□

Using the previous lemma we can construct good interval of any size.

Theorem 3.1. *For every integer c, the interval $[c, c + \lceil\sqrt{c}\,\rceil]$ is good.*

Proof. In order to prove the theorem, it is enough to show that $f(i, j, k, l) \geq 0$ whenever $i, j, k, l \in [c, c + \lceil\sqrt{c}\,\rceil]$. So suppose in contrary that for some i, j, k, l from this interval $f(i, j, k, l) < 0$. By Lemma 2.3, without loss of generality we can assume that $i < k \leq l < j$. Now, let $k = i + s$, $l = i + t$, $j = i + q$ where $0 < s \leq t < q \leq \lceil\sqrt{c}\,\rceil$. Now

$$\frac{1}{k} + \frac{1}{l} = \frac{2i + s + t}{(i + s)(i + t)} \qquad \text{and} \qquad \frac{1}{i} + \frac{1}{j} = \frac{2i + q}{i(i + q)}.$$

If $ij > kl$, then by Lemma 3.1 $s + t < q$. Hence $st < \frac{q^2}{4}$. By Lemma 2.2, $f(i, j, k, l) < 0$, if $\frac{1}{k} + \frac{1}{l} < \frac{1}{i} + \frac{1}{j}$. Hence

$$\begin{aligned}
\frac{2i + s + t}{(i + s)(i + t)} &< \frac{2i + q}{i(i + q)} \\
(2i + s + t)(i^2 + iq) &< (2i + q)(i^2 + (s + t)i + st) \\
2i^3 + (s + t + 2q)i^2 + (s + t)iq &< 2i^3 + (2s + 2t + q)i^2 + 2sti + (s + t)iq + stq \\
i^2\, q &< (s + t)\, i^2 + 2s\,t\,i + s\,t\,q \\
i^2\, q &< (q - 1)\, i^2 + 2s\,t\,i + s\,t\,q,
\end{aligned}$$

from here

$$\begin{aligned}
i^2 &< 2s\,t\,i + s\,t\,q \\
&< 2\frac{q^2}{4}\, i + \frac{q^3}{4},
\end{aligned}$$

which is clearly impossible since $q \leq \lceil\sqrt{i}\,\rceil$.

Similarly, if $ij < kl$, then $s + t > q$. The function f in $f(i, j, k, l)$ is negative if and only if $\frac{1}{i} + \frac{1}{j} < \frac{1}{k} + \frac{1}{l}$. The last inequality implies

$$\begin{aligned}
i^2\, q &> (s + t)\, i^2 + 2s\,t\,i + s\,t\,q \\
&> (q + 1)\, i^2 + 2s\,t\,i + s\,t\,q,
\end{aligned}$$

and obviously this is impossible.

So $f(i, j, k, l) \geq 0$, for arbitrary i, j, k, l from the interval $[c, c + \lceil\sqrt{c}\,\rceil]$. □

Theorem 3.1 is best in the sense that for $c = 2$ the interval $[2, 4]$ is good, but the interval $[2, 5]$ is not. The following corollary is an immediate consequence of the above theorem.

Corollary 3.1. *There are arbitrary long good intervals.*

4 Graphs of maximum degree at least 5

As we already mentioned, the inequality (1) holds for chemical graphs, but not in general. In [10, 17], an examples of connected simple graph G are given such that $M_1/n > M_2/m$. What strikes the eye in these counterexamples is that the maximum vertex degree Δ is 10, or 12 in the second example. So far nothing is said about graphs with maximum vertex degree $\Delta \geq 5$ and $\Delta \notin \{10, 12\}$.

We now produce for any $\Delta \geq 5$ an infinite family of counterexamples to (1) of maximal degree Δ.

Theorem 4.1. *There exists infinitely many graphs G of maximum degree l for which*

$$\frac{M_1}{n} > \frac{M_2}{m}.$$

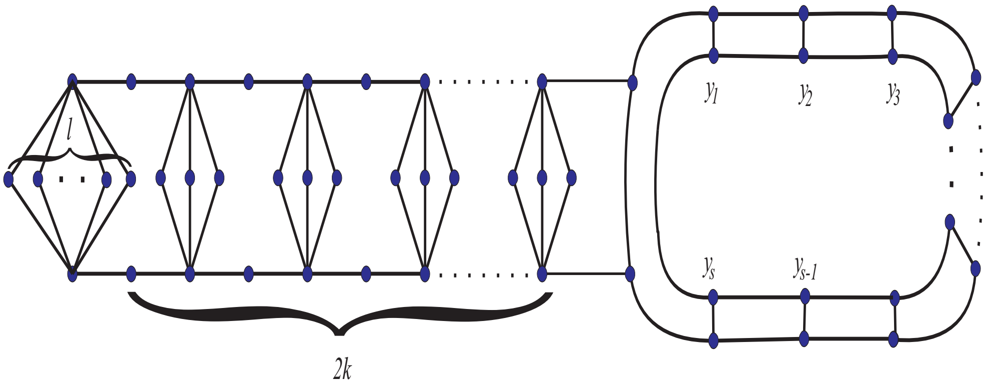

Figure 2: $G(l, k, s)$

Proof. Let G be the graph shown on the Figure 2. This graph has $2k$ vertices of degree 5, $2s + 2$ of degree 3, $5k + l$ vertices of degree 2 and two vertices of degree $l + 1$. Also $m_{5,2} = 10k - 2$, $m_{3,3} = 3s + 2$, $m_{3,5} = 2$ and $m_{l+1,2} = 2(l + 1)$. Then $n = 7k + 2s + l + 4$, $m = 10k + 3s + 2l + 4$, $M_1 = 2(35k + 9s + l^2 + 4l + 10)$, $M_2 = 100k + 27s + 4l^2 + 8l + 52$. From here one can obtained that

$$mM_1 - nM_2 = -2l^2 s + k(-144 + 64l - 8l^2 + s) - 8(6 + 5s) + l(8 + 17s).$$

For every l, we can find k and s big enough such that $mM_1 - nM_2 > 0$. Obviously, we can find infinitely many such pair (k, s). $\square$

Observe that the right side of the graph $G(l, k, s)$ is the cubic graph $K_2 \square C_s$ with one edge twice subdivided. This graph can be substituted with any other cubic graph of appropriate size. $G(4, 9, 33)$ is the smallest graph for which the inequality of Proposition 4.1 holds, and it has 137 vertices.

5 An alternative proof for trees and unicyclic graphs

In [17] is given a proof that inequality (1) holds for trees. Here, the same result is proven in a slightly shorter way. Also an alternative proof for unicyclic graphs [19] is presented.

Let $p_3(G)$ be the number of 3-paths in G, $p_2(G)$ the number of 2-paths, and $C_3(G)$ is the number of 3-cycles. Note that

$$p_3(G) + 3C_3(G) = \sum_{uv\in E} (d(v) - 1)(d(u) - 1), \tag{4}$$

where in the counting uv is the middle edge of the $(d(u) - 1)\,(d(v) - 1)$ corresponding 3-paths. Obviously, such a 3-path corresponds to a 3-cycle when its endvertices coincide.

Theorem 5.1. *For any tree G, it holds $\frac{M_1}{n} \le \frac{M_2}{m}$.*

Proof. If G is a k-star, then $M_1 = kn$ and $M_2 = km$, by which we have equality in (1). So assume now that G has at least two internal adjacent vertices u and v and that v is the only internal neighbor of u. Observe that $M_1 = \sum_{v\in V} d(v)^2 = 2(p_2(G) + m)$. We have

$$M_2 = \sum_{uv\in E} \Big[(d(v) - 1)(d(u) - 1) + (d(u) + d(v)) - 1\Big] = p_3(G) + M_1 - m. \tag{5}$$

Now, since $m = n - 1$, we obtain

$$\begin{aligned} (n-1)M_1 &\le nM_2 \\ (n-1)M_1 &\le n\,[p_3(G) + M_1 - (n-1)] \\ 0 &\le p_3(G) + \frac{2}{n}\,(p_2(G) + (n-1)) - (n-1). \end{aligned}$$

Obviously, $p_2(G) \ge 1$. We will prove now that $p_3(G) \ge n - 3$, and this will establish the theorem. Let $l_1, \ldots, l_k$ be the leaves adjacent to u, and let $w \ne u$ be a neighbor of v. To any vertex x at distance at least 2 from u we associate the 3-path built from the first three edges of the shortest path from x to l_1. To any leaf l_i, $(i \ne 1)$, we associate the path from w to l_i. These 3-paths being all different, we associated a copy of P_3 to any vertex except three, namely l_1, u, v, which ensures that $p_3(G) \ge n - 3$. □

Theorem 5.2. *For any unicyclic graph G, it holds $\frac{M_1}{n} \le \frac{M_2}{m}$.*

Proof. Let $C = x_1x_2 \cdots x_lx_1$ be the unique cycle of G. From (4) and the left equality of (5), we have

$$M_2 = p_3(G) + 3C_3(G) + M_1 - m.$$

Since G is an unicyclic graph, $m = n$. Now, the inequality (1) is equivalent to $M_1 \le M_2$, and hence $M_1 \le p_3(G) + 3C_3(G) + M_1 - n$. And, it is equivalent to

$$n \le p_3(G) + 3C_3(G). \tag{6}$$

Now, remove the edge x_1x_2 from the cycle. Then $G - \{x_1x_2\}$ is a tree and $p_3(G - \{x_1x_2\}) \ge n - 3$. If C is a 3-cycle, then it is obvious that (6) holds. Now, assume $l \ge 4$. Then as it is shown in Theorem 5.1 the graph G has all the 3-paths of $G - \{x_1x_2\}$, and besides them G has at least three more paths: $x_1x_2x_3x_4$, $x_lx_1x_2x_3$, $x_{l-1}x_lx_1x_2$. So, $p_3(G) \ge n$. □

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