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Graph Classes (Dis)satisfying the Zagreb Indices Inequality

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Abstract

Recently Hansen and Vukičević [11] 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 [23] proved that this also holds for trees. In both works a distinct counterexample is given 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 connected graphs of maximum degree Δ, such that the inequality is false.

1 Introduction

The first and second Zagreb indices are among the oldest topological indices [2, 8, 10, 14, 21], defined in 1972 by Gutman and Trinajstić [9], and are given different names in the literature,

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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 exhibit a potential applicability for deriving multi-linear regression models. The article [18] was responsible for a new research wave concerning Zagreb indices.

In the following, 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 often use M_1 and M_2 instead of $M_1(G)$ and $M_2(G)$, respectively. See [6, 7, 16, 12, 26, 27, 28] 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.

One can see that this relation becomes an equality on regular graphs, but also when G is a star. Besides, the inequality is true for trees [23], graphs of maximum degree four, so called chemical graphs [11] and unicyclic graphs [25], even though it does not hold for general graphs. See [11, 23, 5, 13, 20] for various examples of graphs dissatisfying the inequality (1).

In this article, we present some other classes of graphs with prescribed degrees for which (1) holds, and more generally conditions on the distribution of degrees in a graph G implying the relation (1). We also show that there are arbitrarily long intervals $[a, b]$ such that a graph with minimal degree at least a and maximum degree at most b satisfies the same relation. Namely, every graph G, such that its vertex degrees are in the interval $[c, c + \lceil \sqrt{c}\, \rceil]$ for any integer c, satisfies this inequality. We also prove that for any $\Delta \geq 5$, there is an infinite family of connected graphs of maximum degree Δ such that the inequality is false.

We denote by $K_{a,b}$ the *complete bipartite* graph with a vertices in one class and b vertices in the other one. We call *k-star* the star on k edges, and *k-path* the path of length k. Since we discuss necessary conditions for (1) to hold, 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. Then, as shown in [11]:

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

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). In order to simplify (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 as

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

2 Some properties of f

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

Lemma 2.1. *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* $\frac{1}{k} + \frac{1}{l} > \frac{1}{i} + \frac{1}{j}$.

Proof. This result follows immediately by the decomposition of f. Namely

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

□

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

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

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 2.1(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 2.1(a). So, the 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 2.1 (a). So, we conclude that $i < k$. 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 that $k \leq i$. Applying a similar argument as above, one obtains that $k < i \leq j < l$ is the only possible ordering. □

3 Small good sets

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 wonder 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. We give a direct short proof avoiding using the properties of the function f.

Proposition 3.1. *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 that $m_{i,j} = 0$, whenever $i, j \notin \{x, y\}$. By (2), we infer

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

which establishes the claim. □

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 the sets D with property that for every graph G with $D(G) \subseteq D$ the inequality (1) holds. Hence, 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.

In Proposition 3.1 we have shown that for a graph G with $|D(G)| = 2$, the inequality (1) holds. Sun and Chen [19] showed that any graph G with $\Delta(G) - \delta(G) \leq 2$ satisfies (1). Thus, any interval of length three is good. One can generalize this result in the following way:

Proposition 3.2. *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 2.2, 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 $\dfrac{M_2}{m} - \dfrac{M_1}{n} = \sum\limits_{\substack{i \le j, k \le l \\ (i,j),(k,l) \in \mathbb{N}^2}} f(i,j,k,l)\, m_{i,j}\, m_{k,l} > 0$. □

Notice that the above result cannot be extended to any interval of length 4 as Sun and Chen [19] gave a non-connected counterexample. For connected one, consider the graph $G(l,k,s)$ with $l = 4$ from Fig. 2. It is obvious that $D(G(4,k,s))$ 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 5.1. Both graphs contain vertices of degree 2. It is interesting that Sun and Chen [19] proved that any graph G with $\Delta(G) - \delta(G) \le 3$ and $\delta(G) \ne 2$ satisfy (1). Thus, any interval $[x, x+3]$ is good with only exception of $[2,5]$.

The proof of Proposition 3.2 motivates a more general conclusion.

Proposition 3.3. *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 2.2 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 Fig. 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 $K_{b,b}$.
- Choose an edge from the first $K_{a,c}$ graph and 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,

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

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 Fig. 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.

□

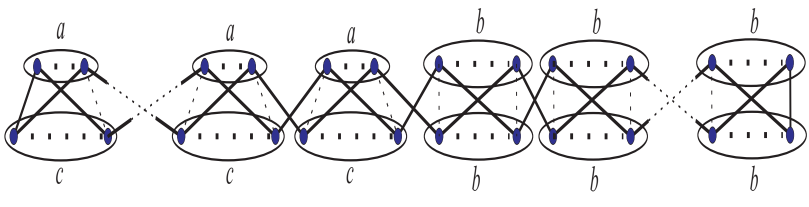

Figure 1: A connected graph G with $D(G) = \{a,b,c\}$. The edges that should be removed are drown with dashed lines.

4 Long good intervals

Our next goal is to determine long good intervals. We will need the following lemma to prove Theorem 4.1.

Lemma 4.1. *For integers c, i, j, and $p \le \lceil\sqrt{c}\,\rceil$ holds:*

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

Proof. First notice that $ij \le \frac{(i+j)^2}{4}$. 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

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

This argument completes the proof. □

Using the previous lemma we can construct good intervals of any size. Notice that the following result holds for $c \le 9$ by the results of Sun and Chen [19] mentioned in the previous section, as in these cases the considered interval is of length at most 4.

Theorem 4.1. *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 $f(i,j,k,l) \ge 0$ whenever i, j, k, $l \in [c, c+\lceil\sqrt{c}\,\rceil]$. Suppose in contrary that for some i, j, k, l from this interval $f(i,j,k,l) < 0$. By Lemma 2.2, without loss of generality we can assume that $i < k \le l < j$. Now, let $k = i+s$, $l = i+t$, $j = i+q$ where $0 < s \le t < q \le \lceil\sqrt{c}\,\rceil$. 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 4.1 $s+t < q$. Hence $st < \frac{q^2}{4}$. By Lemma 2.1, $f(i,j,k,l) < 0$, 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 $q \le \lceil \sqrt{i}\,\rceil$.

Similarly, if $ij<kl$, then $s+t \ge q$. 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

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

and obviously this is impossible.

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

Theorem 4.1 is best in the sense that for $c=2$ the interval $[2,4]$ is good, but the interval $[2,5]$ is not. The following corollaries are immediate consequences of the above theorem.

Corollary 4.1. *If G is a graph with $\Delta(G)-\delta(G)\le\lceil\sqrt{c}\,\rceil$ and $\delta(G)\ge c$ for some integer c, then G satisfies the inequality (1).*

Corollary 4.2. *There are arbitrary long good intervals.*

5 Graphs of maximum degree at least 5

As we already mentioned, the inequality (1) holds for chemical graphs, but not in general. In [11, 23, 5, 13, 20, 19], 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 either the maximum vertex degree is at least 10 or the graph is disconnected. We now produce for each $\Delta \geq 5$ an infinite family of connected planar counterexamples to (1) of maximum degree Δ.

Theorem 5.1. *There exists infinitely many graphs G of maximum degree ≥ 5 for which*

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

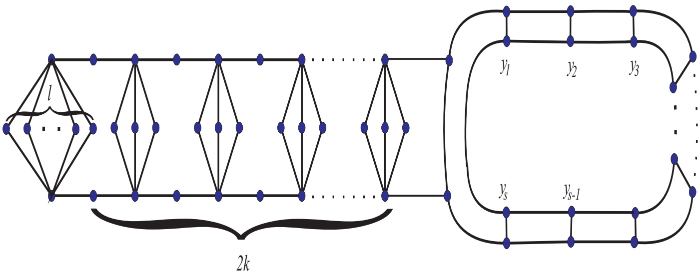

Figure 2: $G(l,k,s)$

Proof. Let G be the graph shown on the Fig. 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 $n = 7k+2s+l+4$, $m = 10k+3s+2l+4$, $M_1 = 2(35k+9s+l^2+4l+10)$, $M_2 = 100k+27s+4l^2+8l+32$. 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). □

Observe that the right side of the graph $G(l,k,s)$ is the cubic graph $K_2 \Box C_s$ 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 Theorem 5.1 holds, and it has 137 vertices.

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