

ON COMPARING ZAGREB INDICES *

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Abstract

Let $G = (V, E)$ be a simple graph with $n = |V|$ vertices and $m = |E|$ edges. The first and second Zagreb indices are among the oldest and the most famous topological indices, defined as $M_1 = \sum_{i \in V} d_i^2$ and $M_2 = \sum_{(i,j) \in E} d_i d_j$, where d_i denote the degree of vertex i . Recently proposed conjecture $M_1/n \leq M_2/m$ has been proven to hold for trees, unicyclic graphs and chemical graphs, while counterexamples were found for both connected and disconnected graphs. Our goal is twofold, both in favor of a conjecture and against it. Firstly, we show that the expressions M_1/n and M_2/m have the same lower and upper bounds, which attain equality for and only for regular graphs. We also establish sharp lower bound for variable first and second Zagreb indices. Secondly, we show that for any fixed number $k \geq 2$, there exists a connected graph with k cycles for which $M_1/n > M_2/m$ holds, effectively showing that the conjecture cannot hold unless there exists some kind of limitation on the number of cycles or the maximum vertex degree in a graph. In particular, we show that the conjecture holds for subdivision graphs.

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1 Introduction

Let $G = (V, E)$ be a simple graph with $n = |V|$ vertices and $m = |E|$ edges. The first Zagreb index M_1 and the second Zagreb index M_2 of G are defined as follows:

$$M_1 = \sum_{i \in V} d_i^2 \quad \text{and} \quad M_2 = \sum_{(i,j) \in E} d_i d_j,$$

where $d_1, d_2, \dots, d_n$ are vertex degrees, while $d_i d_j$ represents weight associated to the edge (i, j) . The Zagreb indices were first introduced in [4] and the survey of properties of M_1 and M_2 is given in [9]. Note that in random graphs with n vertices and uniform edge probability p , the order of magnitude of M_1 is $O(n^3 p^2)$, while the order of magnitude of M_2 is $O(n^4 p^3)$, implying that M_1/n and M_2/m have the same order of magnitude $O(n^2 p^2)$. This led to the following conjecture posed in [6]:

Conjecture 1.1 *For all simple connected graphs G :*

$$\frac{M_1}{n} \leq \frac{M_2}{m},$$

and the bound is tight for complete graphs.

It was shown in [6] that this conjecture is not true in general by finding a disconnected counterexample consisting of a six-vertex star and a triangle, and a connected counterexample on 46 vertices and 110 edges. Nevertheless, it was proven in [6] that the conjecture holds for chemical graphs. Further, it was proven in [11] that the conjecture holds for trees (with equality attained for and only for stars), while in [7] it was proven that the conjecture holds for connected unicyclic graphs (with equality attained for and only for cycles).

Our goal here is twofold, both in favor of a conjecture and against it:

- (i) We show that the expressions M_1/n and M_2/m are both bounded with $\frac{4m^2}{n^2}$ from below and with $\frac{\Delta M_1}{2m}$ from above, with equality attained for and only for regular graphs. We also establish lower bounds for variable Zagreb indices.
- (ii) We show that for any fixed number $k \geq 2$, there exists a connected graph with k cycles for which $M_1/n > M_2/m$ holds, effectively showing that the conjecture cannot hold unless there exists some kind of limitation on the number of cycles or the maximum vertex degree in a graph. In particular, we prove that the conjecture holds for subdivision graphs.

2 Common lower and upper bounds

The following two theorems give sharp lower bounds for M_1 and M_2 . Recall that for a graph with n vertices and m edges, the average value of vertex degrees is $2m/n$.

Theorem 2.1 *It holds that $M_1 \geq \frac{4m^2}{n}$. The equality is attained if and only if graph is regular.*

Proof: We use the Cauchy-Schwartz inequality on vectors $(d_1, d_2, \dots, d_n)$ and $(1, 1, \dots, 1)$ to get

$$M_1 \cdot n = (d_1^2 + d_2^2 + \dots + d_n^2) (1^2 + 1^2 + \dots + 1^2) \geq (d_1 \cdot 1 + d_2 \cdot 1 + \dots + d_n \cdot 1)^2 = (2m)^2.$$

Equality holds if and only if $d_1 = d_2 = \dots = d_n$, namely if and only if G is regular. □

Lemma 2.2 For positive real numbers $x_1, x_2, \dots, x_n$ the following inequality holds:

$$x_1 \ln x_1 + x_2 \ln x_2 + \dots + x_n \ln x_n \geq (x_1 + x_2 + \dots + x_n) \ln \frac{x_1 + x_2 + \dots + x_n}{n}. \quad (1)$$

Proof: The function $f(x) = x \ln x$ is strictly convex on interval $(0, +\infty)$, since its second derivative $f''(x) = \frac{1}{x}$ is positive. The inequality (1) follows directly from the Jensen's inequality [5]

$$\frac{f(x_1) + f(x_2) + \dots + f(x_n)}{n} \geq f\left(\frac{x_1 + x_2 + \dots + x_n}{n}\right).$$

Equality holds in (1) if and only if all x_i are equal. □

Theorem 2.3 It holds that $M_2 \geq \frac{4m^3}{n^2}$. The equality is attained if and only if graph is regular.

Proof: First we use the inequality between the arithmetic and the geometric mean:

$$\frac{M_2}{m} = \frac{\sum_{(i,j) \in E} d_i d_j}{m} \geq \sqrt[m]{\prod_{(i,j) \in E} d_i d_j} = \sqrt[m]{\prod_{i=1}^n d_i^{d_i}}.$$

Since $d_i \geq 1$, we take the natural logarithm of both sides to get

$$\ln \frac{M_2}{m} \geq \frac{1}{m} \sum_{i=1}^n d_i \ln d_i.$$

Then from Lemma 2.2 we get:

$$\ln \frac{M_2}{m} \geq \frac{1}{m} \left(\sum_{i=1}^n d_i \right) \ln \left(\frac{\sum_{i=1}^n d_i}{n} \right) = \frac{1}{m} 2m \ln \frac{2m}{n} = 2 \ln \frac{2m}{n},$$

and finally

$$M_2 \geq \frac{4m^3}{n^2}.$$

Equality holds if and only if $d_1 = d_2 = \dots = d_n$, i.e., if and only if G is regular. □

From two previous theorems, we see that the expressions from Conjecture 1.1 have common sharp lower bound:

$$\frac{4m^2}{n^2} \leq \frac{M_1}{n} \quad \text{and} \quad \frac{4m^2}{n^2} \leq \frac{M_2}{m}.$$

Next we show that these expressions also have common sharp upper bound.

Proposition 2.4 Let Δ be the maximum vertex degree in G . Then

$$\frac{M_1}{n} \leq \frac{\Delta M_1}{2m} \quad \text{and} \quad \frac{M_2}{m} \leq \frac{\Delta M_1}{2m}.$$

Equality is attained simultaneously in both inequalities if and only if G is regular.

Proof: The first inequality is equivalent to the obvious inequality $2m \leq \Delta n$, while the second inequality is equivalent to $2M_2 \leq \Delta M_1$. Then

$$2M_2 = \sum_{(i,j) \in E} 2d_i d_j \leq \sum_{(i,j) \in E} (d_i^2 + d_j^2) = \sum_{i \in V} d_i \cdot d_i^2 \leq \sum_{i \in V} \Delta d_i^2 = \Delta M_1.$$

Equality is attained in both inequalities simultaneously if and only if $d_i = \Delta$ for every $1 \leq i \leq n$, i.e., if and only if G is regular. $\square$

Now, using the upper bound on M_1 from [2] (where Δ is the maximum, while δ is the minimum vertex degree):

$$M_1 \leq m \left(\frac{2m}{n-1} + \frac{n-2}{n-1} \Delta + (\Delta - \delta) \left(1 - \frac{\Delta}{n-1} \right) \right),$$

with equality if and only if G is a star graph or a regular graph or $K_{\Delta+1} \cup (n - \Delta - 1)K_1$, we see that the expressions M_1/n and M_2/m also have common upper bound in terms of n , m , Δ and δ :

$$\begin{aligned} \frac{M_1}{n} &\leq \frac{\Delta}{2} \left(\frac{2m}{n-1} + \frac{n-2}{n-1} \Delta + (\Delta - \delta) \left(1 - \frac{\Delta}{n-1} \right) \right), \\ \frac{M_2}{m} &\leq \frac{\Delta}{2} \left(\frac{2m}{n-1} + \frac{n-2}{n-1} \Delta + (\Delta - \delta) \left(1 - \frac{\Delta}{n-1} \right) \right). \end{aligned}$$

Equality is attained simultaneously in above inequalities if and only if G is regular.

These indices have been generalized to variable first and second Zagreb indices defined as

$${}^\lambda M_1 = \sum_{i=1}^n d_i^{2\lambda} \quad \text{and} \quad {}^\lambda M_2 = \sum_{(i,j) \in E} (d_i d_j)^\lambda$$

More results about comparing variable Zagreb indices can be found in [10] and [12]. For $2\lambda \geq 1$, we define $p = 2\lambda$ and $q = \frac{2\lambda}{2\lambda-1}$ in order to establish relation $\frac{1}{p} + \frac{1}{q} = 1$. Now we use Hölder inequality [5] on vectors $(d_1, d_2, \dots, d_n)$ and $(1, 1, \dots, 1)$ to get

$$\left(\sum_{i=1}^n d_i^p \right)^{1/p} \cdot \left(\sum_{i=1}^n 1^q \right)^{1/q} \geq \sum_{i=1}^n (d_i \cdot 1).$$

Next, raise each side of equation to the power of 2λ

$$\left(\sum_{i=1}^n d_i^{2\lambda} \right) \cdot n^{2\lambda-1} \geq (2m)^{2\lambda}.$$

The last inequality is equivalent with

$${}^\lambda M_1 \geq n \left(\frac{2m}{n} \right)^{2\lambda}.$$

For the variable second Zagreb index and every $\lambda \geq 0$ it holds

$$\frac{{}^\lambda M_2}{m} = \frac{\sum_{(i,j) \in E} (d_i d_j)^\lambda}{m} \geq \sqrt[m]{\prod_{(i,j) \in E} (d_i d_j)^\lambda} = \sqrt[m]{\prod_{i=1}^n d_i^{\lambda d_i}}.$$

We can use the same technique as in the proof of Theorem 2.3 and get lower bound:

$$\lambda M_2 \geq m \left(\frac{2m}{n} \right)^{2\lambda}.$$

Also, we have similar upper bounds for variable Zagreb indices:

$$\frac{\lambda M_1}{n} \leq \frac{\Delta \cdot \lambda M_1}{2m} \quad \text{and} \quad \frac{\lambda M_2}{m} \leq \frac{\Delta \cdot \lambda M_1}{2m}.$$

3 Counterexamples

Let $C(a, b)$ be a graph that is composed of $(a + 1)$ -vertex star with exactly b triangles attached in line at arbitrary leaf (see Figure 1). If triangles have vertex labels v_i, u_i, w_i , where $1 \leq i \leq k$, then there exist edges $u_i v_{i+1}$ for every $1 \leq i \leq k - 1$, and vertex v_1 is connected with an arbitrary leaf of star S_{a+1} .

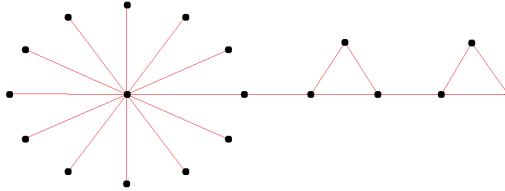


Figure 1: The bicyclic counterexample $C(12, 2)$ with 19 vertices

Assume that $a \geq 3$ and $b \geq 1$. It is obvious that the number of vertices of $C(a, b)$ is $n = a + 3b + 1$ and the number of edges is $m = a + 4b$. Also note that $C(a, b)$ has exactly b cycles.

In $C(a, b)$ there is one vertex of degree a and $a - 1$ pendent vertices. Every triangle has vertex degrees 3, 3, 2, except for the last one which has 3, 2, 2. Now we can calculate the first Zagreb index:

$$M_1(C(a, b)) = a^2 + (a - 1) \cdot 1^2 + 2^2 + (b - 1)(3^2 + 3^2 + 2^2) + (3^2 + 2^2 + 2^2) = a^2 + a + 22b - 2.$$

The weight of $a - 1$ pendent edges is equal to $a \cdot 1$, while every triangle has weights 9, 6, 6, except for the last one which has 6, 6, 4. The edges connecting triangles have weight 9, and therefore,

$$M_2(C(a, b)) = a \cdot 1 \cdot (a - 1) + 2 \cdot a + 2 \cdot 3 + (9 + 6 + 6)(b - 1) + (6 + 6 + 2) + 9(b - 1) = a^2 + a + 30b - 8.$$

The Conjecture 1.1 is equivalent to $M_2 \cdot n - M_1 \cdot m \geq 0$, which for the graph $C(a, b)$ yields:

$$(a^2 + a + 30b - 8)(a + 3b + 1) - (a^2 + a + 22b - 2)(a + 4b) \geq 0.$$

i.e.,

$$a^2(1 - b) + a(7b - 5) + (2b^2 + 14b - 8) \geq 0. \quad (2)$$

Next, fix the number of cycles $b \geq 2$. The left-hand side of (2) is a quadratic function in a . Since the coefficient of a^2 is negative, and the discriminant

$$D = (7b - 5)^2 - 4(1 - b)(2b^2 + 14b - 8) = 8b^3 + 97b^2 - 158b + 57$$

is greater than zero for $b \geq 2$, we get that the left-hand side value of (2) is negative for

$$a > \frac{-(7b-5) + \sqrt{D}}{2(1-b)}. \quad (3)$$

Thus, each value of a satisfying (3) yields a counterexample to Conjecture 1.1 with b cycles. In particular, for $b = 2$ we get that any $a \geq 12$ yields a counterexample to the conjecture and the smallest counterexample of this form is shown in Figure 1.

4 Conclusion

From the previous section it is evident that the Conjecture 1.1 cannot hold unless there exists some kind of limitation on either the maximum vertex degree or the number of cycles in a graph. This *limitation* may be implicitly given, as it becomes evident from the following example.

The subdivision graph $S(G)$ of a graph G is obtained by inserting a new vertex of degree two on each edge of G . If G has n vertices and m edges, then $S(G)$ has $n + m$ vertices and $2m$ edges. Clearly, $S(G)$ is bipartite.

Theorem 4.1 *Let $S(G)$ be a subdivision graph of G . Then,*

$$\frac{M_1(S(G))}{n+m} \leq \frac{M_2(S(G))}{2m},$$

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

Proof: The vertex degrees of G remain the same in the subdivision graph $S(G)$, while the new vertices have degree two. Thus,

$$M_1(S(G)) = M_1(G) + 2^2 \cdot m.$$

Every edge (i, j) of G is subdivided in two parts with weights $2d_i$ and $2d_j$. Therefore,

$$M_2(S(G)) = \sum_{(i,j) \in E} (2d_i + 2d_j) = 2 \sum_{i=1}^n d_i^2 = 2M_1(G).$$

Using these formulas, we get that the inequality $\frac{M_1(S(G))}{n+m} \leq \frac{M_2(S(G))}{2m}$ is equivalent to $\frac{M_1(G)+4m}{n+m} \geq \frac{2M_1(G)}{2m}$, i.e., to $M_1(G) \geq \frac{4m^2}{n}$, which is true by Theorem 2.1. The case of equality easily follows. $\square$

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