On the Classical Zagreb Indices Conjecture of Graphs

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Abstract

The inequality $\frac{M_1(G)}{n(G)} \leq \frac{M_2(G)}{m(G)}$, where $M_1(G)$ and $M_2(G)$ respectively denote the first and the second Zagreb index of a graph G, was originally conjectured to hold for all connected graphs. Although this conjecture has been disproved in general, the inequality remains valid for several important graph families, including trees, unicyclic graphs, and chemical graphs. In this paper, we prove that the inequality holds for every simple graph G satisfying $\delta(G) \geq \frac{n(G)}{2}$. Furthermore, we provide a complete characterization of the extremal cases, showing that equality is attained if and only if G is regular. A quantitative stronger theorem is also deduced.

Keywords: first Zagreb index; second Zagreb index; adjacency matrix; minimum degree

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1 Introduction

In this paper, we consider only finite simple graphs. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. The order and size of G are $n(G) = |V(G)|$ and

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$m(G) = |E(G)|$, respectively. For a vertex $u \in V(G)$, its degree $d_G(u)$ is the number of vertices adjacent to u. The maximum and minimum degrees of G are denoted by $\Delta(G)$ and $\delta(G)$. A graph is regular if $\Delta(G) = \delta(G)$, and biregular if $\Delta(G) \neq \delta(G)$ and its vertex degrees are confined to exactly the two values $\delta(G)$ and $\Delta(G)$. A biregular graph is of class 1 if it contains no edge whose endpoints have the same degree.

A graph with maximum degree at most four is called a chemical graph. The disjoint union of graphs G and H is denoted by $G \cup H$. As usual, K_l, S_l, P_l, and C_l denote the complete graph, star, path, and cycle on l vertices, respectively.

The adjacency matrix A of the graph G is an $n \times n$ matrix whose entries A_{ij} are defined as:

$$A_{ij} = \begin{cases} 1 & \text{if there is an edge from vertex } v_i \text{ to vertex } v_j, \\ 0 & \text{otherwise.} \end{cases}$$

Gutman and Trinajstić [13, 14] introduced the first and second Zagreb indices:

$$M_1(G) = \sum_{v \in V(G)} d_G(v)^2, \qquad M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v).$$

The Zagreb indices are among the most thoroughly studied degree-based graph invariants; we refer the reader to [2, 5, 17–19, 21, 26] and the references therein for further details. In addition, for recent works on Zagreb indices and their connections to other graph parameters see [1, 9–11, 15, 18, 22, 27].

The following conjecture was proposed in the early 2000s.

Conjecture 1. [4, 6, 7] *If G is a connected graph, then*

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

Hansen and Vukičević [16] showed that the conjecture fails for general graphs but holds for chemical graphs. They gave the disconnected counterexample $S_6 \cup C_3$ and a connected counterexample on 46 vertices. Vukičević and Graovac [23] proved the conjecture for trees, with equality iff $G \cong S_{n(G)}$. Liu [20] proved it for unicyclic graphs, with equality iff $G \cong C_{n(G)}$. Using AutoGraphiX, Caporossi, Hansen, and Vukičević [8] found infinite counterexamples with cyclomatic number $\nu(G) = m(G) - n(G) + 1 \geq 2$. Andova et al. [3] proved that every graph with degrees in the interval $[\delta(G), \delta(G) + \lceil \sqrt{\delta(G)} \rceil]$ satisfies the Zagreb inequality. Vukicević et al. [24] characterized graphs with $M_1/n = M_2/m$ (biregular class 1, subdivisions of regular graphs, and infinite unions such as $K_p \cup K_{a,b}$), construct connected non-regular examples of max degree 5 satisfying equality, and give sufficient conditions for unions to preserve the Zagreb inequality/equality. Recently, the first author [12] showed that in the class of graphs with $\Delta(G) - \delta(G) \leq 3$, all counterexamples have $\Delta(G) = 5$ and $\delta(G) = 2$, and infinitely many exist.

In this paper, we study graphs where every vertex is adjacent to at least half of the vertices. We prove that Conjecture 1 holds for such graphs, with equality if and only if the graph is regular. Moreover, we also prove a quantitative stronger result.

2 Main Results

In this section, we establish that Conjecture 1 holds for all graphs whose minimum degree is at least half of their order. Furthermore, we characterize the extremal graphs for which equality is attained.

Theorem 2. *If G is a graph with $\delta(G) \geq \frac{n(G)}{2}$, then*

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

Moreover, equality holds if and only if G is regular.

Proof. Set $n = n(G)$, $m = m(G)$, $M_1 = M_1(G)$, and $M_2 = M_2(G)$. Let $d_1, \dots, d_n$ be the degree sequence of G, and let $\bar{d}$ be the average degree of G, that is,

$$\bar{d} = \frac{2m}{n}.$$

Let A be the adjacency matrix of G, and respectively define the degree vector and the identity vector by

$$\mathbf{d} = (d_1, \dots, d_n)^T, \qquad \mathbf{1} = (1, \dots, 1)^T.$$

We decompose the degree vector into its mean and a deviation:

$$\mathbf{x} = \mathbf{d} - \bar{d}\,\mathbf{1}.$$

Since $\mathbf{1}^T\mathbf{d} = \sum_i d_i = 2m = n\bar{d}$, we have

$$\mathbf{1}^T\mathbf{x} = \mathbf{1}^T(\mathbf{d} - \bar{d}\mathbf{1}) = n\bar{d} - \bar{d}n = 0. \tag{1}$$

Because $A\mathbf{1} = \mathbf{d}$, we obtain the fundamental identity

$$\mathbf{d}^T A\mathbf{d} = 2M_2. \tag{2}$$

Indeed, expanding the quadratic form gives

$$\mathbf{d}^T A\mathbf{d} = \sum_{i=1}^{n}\sum_{j=1}^{n} d_i A_{ij} d_j = \sum_{\substack{i,j=1 \\ ij\in E(G)}}^{n} d_i d_j.$$

For every edge $uv \in E(G)$, the ordered pairs (u, v) and (v, u) both appear in the sum, each contributing $d_u d_v$. Hence each edge contributes exactly $2d_u d_v$, and therefore

$$\mathbf{d}^T A\mathbf{d} = 2\sum_{uv\in E(G)} d(u)d(v) = 2M_2.$$

Similarly, we have

$$\mathbf{d}^T\mathbf{d} = \sum_{i=1}^{n} d_i^2 = M_1. \tag{3}$$

Now, using the decomposition $\mathbf{d} = \bar{d}\mathbf{1} + \mathbf{x}$, we compute:

$$\begin{aligned}\mathbf{d}^T A\mathbf{d} &= (\bar{d}\mathbf{1} + \mathbf{x})^T A(\bar{d}\mathbf{1} + \mathbf{x}) \\ &= (\bar{d})^2\mathbf{1}^T A\mathbf{1} + 2\bar{d}\,\mathbf{1}^T A\mathbf{x} + \mathbf{x}^T A\mathbf{x}.\end{aligned}$$

We know $\mathbf{1}^T A\mathbf{1} = 2m = n\bar{d}$. Also, using (1),

$$\mathbf{1}^T A\mathbf{x} = (A\mathbf{1})^T\mathbf{x} = \mathbf{d}^T\mathbf{x} = (\bar{d}\mathbf{1} + \mathbf{x})^T\mathbf{x} = \bar{d}\,\underbrace{\mathbf{1}^T\mathbf{x}}_{0} + |\mathbf{x}|^2 = |\mathbf{x}|^2.$$

Therefore,

$$\mathbf{d}^T A\mathbf{d} = n(\bar{d})^3 + 2\bar{d}|\mathbf{x}|^2 + \mathbf{x}^T A\mathbf{x}. \tag{4}$$

On the other hand, from $\mathbf{d} = \bar{d}\mathbf{1} + \mathbf{x}$,

$$\mathbf{d}^T\mathbf{d} = |\mathbf{d}|^2 = n(\bar{d})^2 + |\mathbf{x}|^2,$$

so multiplying by $\bar{d}$ gives

$$\bar{d}\,\mathbf{d}^T\mathbf{d} = n(\bar{d})^3 + \bar{d}|\mathbf{x}|^2. \tag{5}$$

Subtracting (5) from (4) and using (2) and (3), we obtain the key identity

$$2M_2 - \bar{d}M_1 = \bar{d}|\mathbf{x}|^2 + \mathbf{x}^T A\mathbf{x}. \tag{6}$$

We now need a lower bound for $\mathbf{x}^T A\mathbf{x}$. Let $\overline{G}$ be the complement of G, with the adjacency matrix $\overline{A}$. Since $A + \overline{A} = J - I$ (where J is the all-ones matrix and I is the identity), and using (1),

$$\mathbf{x}^T A\mathbf{x} = \mathbf{x}^T(J - I - \overline{A})\mathbf{x} = -|\mathbf{x}|^2 - \mathbf{x}^T\overline{A}\,\mathbf{x}. \tag{7}$$

For any vector $\mathbf{y}$, we have $\mathbf{y}^T\overline{A}\,\mathbf{y} \le \Delta(\overline{G})|\mathbf{y}|^2$, because the spectral radius of $\overline{A}$ is at most its maximum degree, cf. [25, Lemma 8.6.18]. Hence

$$\mathbf{x}^T A\mathbf{x} \ge -\big(1+\Delta(\overline{G})\big)|\mathbf{x}|^2. \tag{8}$$

Now observe that

$$\Delta(\overline{G}) = n-1-\delta(G).$$

Under the hypothesis $\delta(G) \ge n/2$, we get

$$1+\Delta(\overline{G}) = n-\delta(G) \le n-\frac{n}{2} = \frac{n}{2}.$$

Substituting this into (8) yields

$$\mathbf{x}^T A\mathbf{x} \ge -\frac{n}{2}|\mathbf{x}|^2. \tag{9}$$

Combining (6) and (9), we obtain the strong quantitative estimate

$$2M_2 - \bar{d}M_1 \ge \left(\bar{d}-\frac{n}{2}\right)|\mathbf{x}|^2. \tag{10}$$

Since

$$\bar{d} = \frac{2m}{n} \ge \delta(G) \ge \frac{n}{2},$$

the coefficient $\bar{d} - n/2$ is nonnegative. Therefore the right-hand side of (10) is nonnegative, and we have

$$2M_2 \ge \bar{d}M_1 = \frac{2m}{n}M_1.$$

Dividing by $2m > 0$ gives

$$\frac{M_1}{n} \le \frac{M_2}{m}. \tag{11}$$

It remains to characterize equality in (11). If G is regular, say $d_i = \bar{d}$ for all i, then a direct computation gives

$$\frac{M_1}{n} = (\bar{d})^2, \qquad \frac{M_2}{m} = (\bar{d})^2,$$

so equality holds in (11).

Conversely, assume that equality holds in (11). Then equality holds in (10), so

$$\left(\bar{d}-\frac{n}{2}\right)|\mathbf{x}|^2 = 0.$$

If $\bar{d} > n/2$, then $|\mathbf{x}|^2 = 0$, which means $\mathbf{d} = \bar{d}\mathbf{1}$, so G is regular. If $\bar{d} = n/2$, then from $\delta(G) \ge n/2 = \bar{d}$ and the fact that $\bar{d}$ is the average degree, we must have $d_i = \bar{d}$ for every vertex; hence G is regular again. Thus equality holds if and only if G is regular. □

We have thus proven our main result. It is certainly worth noting, however, that the proof of Theorem 2 also allows us to obtain the following, stronger result.

Theorem 3. *If G is a graph with $\delta(G) \geq \frac{n(G)}{2}$, and $\bar{d}$ is its average degree, then*

$$2M_2(G) - \bar{d}\, M_1(G) \geq \left(\bar{d} - \frac{n(G)}{2}\right) \sum_{v \in V(G)} \left(d(v) - \bar{d}\right)^2 \geq 0. \tag{I}$$

Proof. Let's use the same abbreviated symbols n, M_1, M_2 as in the proof of Theorem 2, and consider Equation (10) derived in the proof. Since $|\mathbf{x}|^2 = \sum_v (d(v) - \bar{d})^2$, we have

$$2M_2 - \bar{d}M_1 \geq \left(\bar{d} - \frac{n}{2}\right) |\mathbf{x}|^2 = \left(\bar{d} - \frac{n}{2}\right) \sum_{v \in V(G)} (d(v) - \bar{d})^2.$$

Because $\bar{d} \geq \delta(G) \geq n/2$, the factor $\bar{d} - n/2$ is nonnegative, so the right-hand side is indeed ≥ 0. $\square$

Note that Theorem 2 can also be derived as a consequence of Theorem 3. Indeed, by (1) we have $2M_2 - \bar{d}M_1 \geq 0$, which is exactly $M_1/n \leq M_2/m$. Hence, as already mentioned, Theorem 3 is a stronger statement than Theorem 2. Indeed, it gives a precise lower bound on the gap between $2M_2$ and $\bar{d}M_1$ in terms of the variance of the degree sequence.

3 Concluding Remarks

We have established a sharp sufficient condition for the Zagreb inequality

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

to hold, namely that the minimum degree of the graph be at least $n/2$. The result is sharp in the sense that equality is completely characterized: it occurs precisely for regular graphs.

This condition is genuinely restrictive, as the inequality is known to fail for general graphs. The appearance of the threshold $n(G)/2$ is therefore not an artifact of the proof but reflects a genuine structural transition in the behaviour of the Zagreb indices. Graphs satisfying this minimum-degree condition are dense enough that the second Zagreb index dominates the first in the normalized sense expressed by the inequality.

The quantitative estimate obtained in Theorem 3 is notably stronger than the theorem itself. It shows that the gap between $2M_2(G)$ and $\bar{d}M_1(G)$ is at least a nonnegative multiple of the variance of the degree sequence. This suggests that the inequality becomes progressively stronger as the degrees deviate from regularity, and it highlights regularity as the unique extremal case.

Several directions for further investigation naturally arise from this work. It would be interesting to determine whether the threshold $n(G)/2$ can be lowered for graphs belonging to special classes, such as those with bounded clique number, high connectivity, or prescribed chromatic number.

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Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Our manuscript has no associated data.

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