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More on the Zagreb Indices Inequality

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Abstract

The Zagreb indices are very popular topological indices in mathematical chemistry and attracted a lot of attention in recent years. The first and second Zagreb indices of a graph $G = (V, E)$ are defined as $M_1(G) = \sum_{v_i \in V} d_i^2$ and $M_2(G) = \sum_{v_i \sim v_j} (d_i d_j)$, where d_i denotes the degree of a vertex v_i and $v_i \sim v_j$ represents the adjacency of vertices v_i and v_j in G. It has been conjectured that $M_1/n \leq M_2/m$ holds for a connected graph G with $n = |V|$ and $m = |E|$. Later, it is proved that this inequality holds for some classes of graphs but does not hold in general. This inequality is proved to be true for graphs with $d_i \in [h, h + \lceil\sqrt{h}\rceil]$ or $d_i \in [h, h + z]$, where $h \geq z(z-1)/2$. In this paper, we prove that the graphs satisfy the inequality if the sequences (d_i) and (S_i) have the similar monotonicity, where $S_i = \sum_{v_j \in N(v_i)} d_j$ and $N(v_i) = \{v_j \in V | v_i \sim v_j\}$. As a consequence, we present an infinite family of connected graphs with $d_i \in [1, \infty)$, for which the inequality holds. Moreover, we establish the relations between M_1/n and M_2/m in case of general graphs.

1 Introduction

The structural invariants are numerical parameters of a (molecular) graph that characterize its topology and are referred to as topological indices in mathematical chemistry. They are the conclusive outcomes of a mathematical and logical process which converts the chemical knowledge concealed inside the molecule's symbolic representation into a valuable number that has been proved to be fruitful in modeling a variety of physico-chemical properties in various QSAR and QSPR investigations [7, 17, 23].

We consider simple, finite and undirected graph $G = (V, E)$ having vertex set $V =$

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$\{v_1, v_2, \ldots, v_n\}$ and edge set E, where $n = |V|$ and $m = |E|$ referred to as order and size of G, respectively. For a vertex $v_i \in V$, we denote by $N(v_i)$, the set of vertices that are adjacent to v_i and by $d_i = |N(v_i)|$, the degree of v_i. Also, we denote the maximum degree and the minimum degree by Δ and δ respectively. We assume that the degree sequence $(d_i) = (d_1, d_2, \cdots, d_n)$ satisfies $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta > 0$. If this sequence is constant, i.e., $d_i = \delta = \Delta$, for every vertex v_i in G, then G is called a regular graph. Further, for a given vertex v_i, we define $S_i = \sum_{v_i \sim v_j} d_j$ and we call $(S_i) = (S_1, S_2, \cdots, S_n)$ a degree-sum sequence. It is easy to observe that $\delta^2 = \min_{v_i \in V}\{S_i\}$ and $\Delta^2 = \max_{v_i \in V}\{S_i\}$.
The Zagreb indices (ZIs) are among the oldest, best known, and most studied vertex degrees-based topological indices which were put forward in [9]. Later, they were enhanced in [10] and utilized in the modeling of structure-property relationship [23]. The first and second ZIs $M_i(G)$ $(i = 1, 2)$ of G are respectively defined as:

$$M_1(G) = \sum_{i=1}^{n} d_i^2$$

and

$$M_2(G) = \sum_{v_i \sim v_j} d_i d_j.$$

Although the Zagreb indices were introduced at the same time and were almost always studied together, the comparison between them was not done for several years. Notice that the order of magnitude of M_1 for general graphs is $O(n^3)$, while the order of magnitude of M_2 is $O(mn^2)$. This recommends comparing M_1/n and M_2/m rather than M_1 and M_2. Caporossi and Hansen proposed the following conjecture based on the AutoGraphiX conjecture-generating computer method [5].

Conjecture 1. *For all connected graphs G:*

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

where the bound is tight for complete graphs.

The relationship (1) is often referred to as the Zagreb indices inequality in the literature. Soon after the inequality was announced, it was investigated in [12] that there exist graphs for which (1) fails to hold. Despite of the fact that the work presented in [12] seemed to completely resolve Hansen's conjecture, it was just the origin of a novel platform for researchers to investigate the validity or non-validity of (1) for numerous classes of graphs [1–3,6,8,11,14–16,20–22,24]. The developments on this conjecture are summarized in the survey [18].

The Zagreb indices inequality (1) is proved to hold for graphs having vertex degrees from the set $\{h-z, h, h+z\}$, for any $h, z \in \mathbb{N}$, see [3]. This is equivalent to (1) satisfies for graphs having vertex degrees belong to any interval of length three. Later, in [21], it was proven that any graph G having vertex degrees from an interval $[h, h+3]$, satisfies (1), for any $h \in \mathbb{N}$ but $h \neq 2$. This finding was strengthened in [3] by demonstrating that the inequality (1) attains for graphs having vertex degrees from an interval $[h, h+\lceil\sqrt{h}\rceil]$, for any $h \in \mathbb{N}$. This result was further enhanced in [2], where it was shown that for every $z \in \mathbb{N}$, the inequality (1) attains for graphs having vertex degrees from an interval $[h, h+z]$ if and only if $h \geq z(z-1)/2$ or $[h, h+z] = [1, 4]$.

The question of how to characterize the graphs for which the inequality (1) holds is still unanswered. In this paper, we make a step forward by demonstrating that this inequality holds for graphs with degree sequence (d_i) and degree-sum sequence (S_i) have the similar monotonicity. Resultantly, we present an infinite family of connected graphs with vertex degrees belong to the interval $[1, \infty)$, for which the inequality (1) holds. Moreover, we establish the relations between $M_1(G)/n$ and $M_2(G)/m$ for general graphs.

This paper is organized as follows. In section 2, we compare M_1/n and M_2/m and provide a sufficient condition for the validity of Zagreb indices inequality (1). From this we give an infinite family of connected graphs in section 3, satisfying the Zagreb indices inequality (1). In section 4, we obtain the relations between M_1/n and M_2/m for the general graphs.

2 Comparison between M_1/n and M_2/m

In this section, we prove that the graphs satisfy the Zagreb indices inequality (1) if both the degree sequence and the degree-sum sequence have the similar monotonicity.

Lemma 1. *For any graph G:*

$$M_1(G) = \sum_{i=1}^{n} S_i, \tag{2}$$

where $S_i = \sum_{v_j \in N(v_i)} d_j$.

Proof.

$$\begin{aligned} M_1(G) &= \sum_{i=1}^{n} d_i^2 = \sum_{i=1}^{n} d_i d_i = d_1 d_1 + d_2 d_2 + \cdots + d_n d_n \\ &= \underbrace{d_1 + d_1 + \cdots + d_1}_{d_1 \text{ times}} + \underbrace{d_2 + d_2 + \cdots + d_2}_{d_2 \text{ times}} + \cdots + \underbrace{d_n + d_n + \cdots + d_n}_{d_n \text{ times}} \end{aligned}$$

By rearranging with respect to the sum of degrees of neighbor vertices of each vertex v_i, we have

$$M_1(G) = \sum_{i=1}^{n} \sum_{v_j \in N(v_i)} d_j.$$

By taking $S_i = \sum_{v_j \in N(v_i)} d_j$, the desired result follows. ■

Lemma 2. *For any graph G:*

$$M_2(G) = \frac{1}{2} \sum_{i=1}^{n} d_i S_i, \tag{3}$$

where $S_i = \sum_{v_j \in N(v_i)} d_j$.

Proof.

$$\begin{aligned} M_2(G) &= \frac{1}{2} \sum_{v_i \sim v_j} 2 d_i d_j \\ &= \frac{1}{2} \left[d_1 \sum_{v_j \in N(v_1)} d_j + d_2 \sum_{v_j \in N(v_2)} d_j + \cdots + d_n \sum_{v_j \in N(v_n)} d_j \right] \\ &= \frac{1}{2} \sum_{i=1}^{n} d_i \sum_{v_j \in N(v_n)} d_j. \end{aligned}$$

By setting $S_i = \sum_{v_j \in N(v_i)} d_j$, the required result follows. ■

Lemma 3. *A graph G having order $n = p + q$ and degree-sum sequence $(S_1, S_2, \cdots, S_n)$ is complete bipartite graph if and only if $S_1 = S_2 = \cdots = S_n = pq$.*

Proof. Let G be a complete bipartite graph having $n = p + q$ vertices and bipartition (V_1, V_2), where $|V_1| = p$ and $|V_2| = q$. By the definition of complete bipartite graph, degree of each vertex $p_i \in V_1$ is q and likewise degree of each vertex $q_j \in V_2$ is p. Therefore, for each $p_i \in V_1$, we have

$$S_i = \sum_{q_j \in N(p_i)} d_j = \underbrace{q + q + \cdots + q}_{p \text{ times}} = pq.$$

Also, for each $q_j \in V_2$, we have

$$S_j = \sum_{p_i \in N(q_j)} d_i = \underbrace{p + p + \cdots + p}_{q \text{ times}} = qp.$$

Hence, for every vertex $v_i \in V$, we have $S_1 = S_2 = \cdots = S_n = pq$.

Conversely, let $S_1 = S_2 = \cdots = S_n = pq = k$, where $k \in \mathbb{N}$. Then, we prove that for each value of k, we get a complete bipartite graph $G \cong K_{p,q}$ with the bipartition (V_1, V_2), where $|V_1| = p$ and $|V_2| = q$. For the values of k, three cases arise:

Case 1. If $k = 1$, then $G \cong K_{1,1}$, for which $S_1 = S_2 = 1$.

Case 2. If k is a prime number, then $G \cong K_{1,k}$, for which $S_1 = S_2 = \cdots = S_{k+1} = k$.

Case 3. If k is a composite number, i.e., $k = pq$, then $G \cong K_{p,q}$, for which $S_1 = S_2 = \cdots = S_{p+q} = pq = k$. ■

In the following, we state the well-known Chebyshev's inequality:

Lemma 4. *[13] Let $\xi_1, \xi_2, \ldots, \xi_n$ and $\sigma_1, \sigma_2, \ldots, \sigma_n$ be real numbers. If the sequences (ξ_i) and (σ_i) have the similar monotonicity, then*

$$\frac{1}{n}\sum_{i=1}^{n} \xi_i \sigma_i \geq \left(\frac{1}{n}\sum_{i=1}^{n} \xi_i\right)\left(\frac{1}{n}\sum_{i=1}^{n} \sigma_i\right). \tag{4}$$

The inequality is reversed if the sequences (ξ_i) and (σ_i) have the opposite monotonicity. Equality attains in each case if and only if $\xi_1 = \xi_2 = \cdots = \xi_n$ or $\sigma_1 = \sigma_2 = \cdots = \sigma_n$.

Now, we present the main result of this section.

Theorem 1. *Let G be a connected graph having degree sequence (d_i), degree-sum sequence (S_i), order n and size m. If (d_i) and (S_i) have the similar monotonicity, then*

$$\frac{M_1(G)}{n} \leq \frac{M_2(G)}{m}. \tag{5}$$

Equality attains if and only if G is regular or complete bipartite graph.

Proof. Let $\xi_1, \xi_2, \cdots, \xi_n$ and $\sigma_1, \sigma_2, \cdots, \sigma_n$ be real numbers, satisfying $\xi_1 \leq \xi_2 \leq \cdots \leq \xi_n$ and $\sigma_1 \leq \sigma_2 \leq \cdots \leq \sigma_n$ or $\xi_1 \geq \xi_2 \geq \cdots \geq \xi_n$ and $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$. Then, inequality (4) is valid. We choose $\xi_i = d_i$ and $\sigma_i = S_i$, for which inequality (4) becomes

$$\frac{1}{n}\sum_{i=1}^{n} d_i S_i \geq \left(\frac{1}{n}\sum_{i=1}^{n} d_i\right)\left(\frac{1}{n}\sum_{i=1}^{n} S_i\right).$$

From (2) and (3), we have

$$\frac{2}{n}M_2(G) \geq \frac{2m}{n^2}M_1(G).$$

From here, the required inequality (5) follows.

Since equality in (4) attains if and only if $\xi_1 = \xi_2 = \cdots = \xi_n$ or $\sigma_1 = \sigma_2 = \cdots = \sigma_n$. This means that equality in (5) attains if and only if $d_1 = d_2 = \cdots = d_n$ or $S_1 = S_2 = \cdots = S_n$. Then, $d_1 = d_2 = \cdots = d_n$ implies G is a regular graph or from Lemma 3, $S_1 = S_2 = \cdots = S_n$ implies G is a complete bipartite graph. ■

Remark 1. *For the sufficient condition presented in Theorem 1, the Zagreb indices inequality holds for both connected and non-connected graphs.*

3 Graphs with $d_i \in [1, \infty)$ satisfying the Zagreb indices inequality

Consider the infinite family of connected graphs $G(r,t)$ that is constructed from wheel graphs $W_r \cong C_{r-1} + v$ by adding t pendant edges at a single vertex of cycles C_r, where $r \geq 4$ and $t \leq r-3$. The order and size of $G(r,t)$ are $t+r+1$ and $t+r$ respectively. Observe that $\Delta(G(r,t)) = r < \infty$ and $\delta(G(r,t)) = 1$. Therefore, $d_i \in [1, \infty)$. The graph $G(r,t)$ with labeled vertices is depicted in Fig. 1. We labeled the vertices of $G(r,t)$ in such a way that both the degree sequence $(d_1, d_2, \cdots, d_t, \cdots, d_{t+r-1}, d_{t+r}, d_{t+r+1})$ and the degree-sum sequence $(S_1, S_2, \cdots, S_t, \cdots, S_{t+r-1}, S_{t+r}, S_{t+r+1})$, are monotonically increasing. Hence, from Theorem 1, the Zagreb indices inequality (1) is valid for $G(r,t)$.

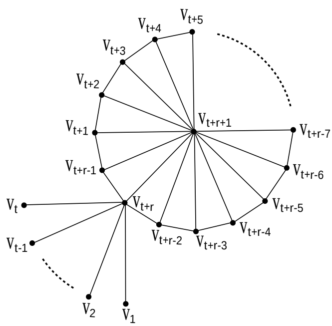

Figure 1. Graph $G(r,t)$.

4 Relations between M_1/n and M_2/m

In this section, we establish the relations between $M_1(G)/n$ and $M_2(G)/m$ for any graph G.

We need the following inequality.

Theorem 2. *[4] Let $\xi_1, \xi_2, \ldots, \xi_n$ and $\sigma_1, \sigma_2, \ldots, \sigma_n$ be positive real numbers such that for $1 \leq i \leq n$, it holds that $r \leq \xi_i \leq R$ and $t \leq \sigma_i \leq T$. Then,*

$$\left| n \sum_{i=1}^{n} \xi_i \sigma_i - \sum_{i=1}^{n} \xi_i \sum_{i=1}^{n} \sigma_i \right| \leq \tau(n)\,(R-r)\,(T-t)\,, \tag{6}$$

where $\tau(n) = n \left\lceil \frac{n}{2} \right\rceil \left(1 - \frac{1}{n} \left\lceil \frac{n}{2} \right\rceil\right)$. Further, equality attains if and only if $\xi_1 = \xi_2 = \cdots = \xi_n$ and $\sigma_1 = \sigma_2 = \cdots = \sigma_n$.

Theorem 3. *Let G be a graph having order n and size m edges, then*

$$-\phi(m,n) + \frac{M_1(G)}{n} \leq \frac{M_2(G)}{m} \leq \frac{M_1(G)}{n} + \phi(m,n), \tag{7}$$

where $\phi(m,n) = \frac{\tau(n)}{2mn} (\Delta - \delta)^2 (\Delta + \delta)$ and $\tau(n) = n \left\lceil \frac{n}{2} \right\rceil \left(1 - \frac{1}{n} \left\lceil \frac{n}{2} \right\rceil\right)$. Further, each inequality achieves if and only if G is a regular.

Proof. Let $\xi_1, \xi_2, \cdots, \xi_n$ and $\sigma_1, \sigma_2, \cdots, \sigma_n$ be positive real numbers for which there exist real constants r, t, R and T, so that for each i, $r \leq \xi_i \leq R$ and $t \leq \sigma_i \leq T$. Then, from Theorem 2, the inequality (6) is valid. We choose $\xi_i = d_i$, $\sigma_i = S_i$, $r = \delta$, $R = \Delta$, $t = \delta^2$, and $T = \Delta^2$, for which the inequality (6) becomes

$$\left| n \sum_{i=1}^{n} d_i S_i - \sum_{i=1}^{n} d_i \sum_{i=1}^{n} S_i \right| \leq \tau(n)(\Delta - \delta)(\Delta^2 - \delta^2),$$

where $\tau(n) = n \left\lceil \frac{n}{2} \right\rceil \left(1 - \frac{1}{n} \left\lceil \frac{n}{2} \right\rceil\right)$.
From (2) and (3), we have

$$|2nM_2(G) - 2mM_1(G)| \leq \tau(n)(\Delta - \delta)^2(\Delta + \delta).$$

This implies that

$$-\tau(n)(\Delta - \delta)^2(\Delta + \delta) + 2mM_1(G) \leq 2nM_2(G) \leq 2mM_1(G) + \tau(n)(\Delta - \delta)^2(\Delta + \delta).$$

By taking $\phi(m,n) = \frac{\tau(n)}{2mn} (\Delta - \delta)^2 (\Delta + \delta)$, the required compound inequality (7) follows. Since equality achieves in (6) if and only if $\xi_1 = \xi_2 = \cdots = \xi_n$ and $\sigma_1 = \sigma_2 = \cdots = \sigma_n$. This means that each equality achieves in (7) if and only if $d_1 = d_2 = \cdots = d_n$ and $S_1 = S_2 = \cdots = S_n$. This implies that G is a regular. ■

5 Conclusion

This paper is to study a new sufficient condition for the validity of Zagreb indices inequality (1) and to establish relations between $M_1(G)/n$ and $M_2(G)/m$ for the general graphs. The main contribution of this paper deals with the validity of inequality (1) for the graphs with vertex degrees belong to an interval of any length. We would like to conclude this paper by raising the following question:

Problem: Characterize the graphs for which both the degree sequence (d_i) and the degree-sum sequence (S_i) have the similar monotonicity.

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