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UPPER BOUNDS FOR ZAGREB INDICES OF CONNECTED GRAPHS[1]

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Abstract

For a (molecular) graph, the first Zagreb index M_1 is equal to the sum of squares of the vertex degrees, and the second Zagreb index M_2 is equal to the sum of products of degrees of pairs of adjacent vertices. New upper bounds for M_1 and M_2 of connected graphs are obtained, in terms of the number of vertices, number of edges, and diameter.

INTRODUCTION

Let $G = (V, E)$ be a simple graph with vertex set $V = \{1, 2, \ldots, n\}$, and edge set E, such that $|E| = m$. Sometimes we refer to G as an (n, m) graph. For $i, j \in V$, if i is adjacent to j then we write $i \sim j$, otherwise $i \not\sim j$. The degree of the vertex i is denoted by d_i or $d(i)$.

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In what follows $D = D(G)$ and $g(G)$ denote the diameter (the greatest distance between two vertices) and the girth (the size of the smallest cycle), respectively, of G.

For a graph G, the first and the second Zagreb indices, M_1 and M_2, respectively, are defined as:

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

$$M_2 = M_2(G) = \sum_{i \sim j} d_i \, d_j \, .$$

The Zagreb indices M_1 and M_2 were introduced in [1,2]. They reflect the extent of branching of the underlying molecular structure [1–5]. Their main properties were recently summarized in [6–8]. Also recently, numerous bounds for M_1 and M_2 were obtained [7–15].

In this note, we focus our attention on connected graphs and offer a few new upper bounds for M_1 and M_2 in terms of the number of vertices (n), number of edges (m), and graph diameter (D).

UPPER BOUNDS FOR M_1

Up to now, several upper bounds for M_1 in terms of m and n have been obtained:

Theorem A [9]. $M_1(G) \leq m(m+1)$, with equality attained, for example, by $K_{1,n-1}$ and K_3.

Theorem B [9–11]. $M_1(G) \leq m\,[2\,m/(n-1) + n - 2]$, with equality holding if and only if $G \cong K_n$ or $G \cong K_{1,n-1}$ or $G \cong K_1 \cup K_{n-1}$.

Theorem C [12]. $M_1(G) \leq n\,(2m - n + 1)$, with equality holding if only if $G \cong K_n$ or $G \cong K_{1,n-1}$ or $G \cong m\,K_2$.

Theorem D [12]. Let G be a triangle-free (n,m) graph. Then $M_1(G) \leq m\,n$.

In this paper we consider connected graphs and first establish the following Lemmas.

Lemma 1. Let $G = (V,E)$ be a connected (n,m) graph with $n > 3$. Then $M_1(G) = m(m+1)$ if and only if $G \cong K_{1,n-1}$.

Proof. If $M_1(G) = m(m+1)$, then for any $\{i,j\} \in E$

$$d(i) + d(j) = m + 1 \ . \tag{1}$$

Suppose that the opposite is true and assume that there exists an edge $\{u_1, v_1\} \in E$, such that $d(u_1) + d(v_1) \neq m+1$. For obvious reasons, for all $\{u,v\} \in E$, it must be $d(u) + d(v) \leq m+1$. Thus, our assumption is that $d(u_1) + d(v_1) < m+1$.

If so, then we have

$$\sum_{u \sim v} [d(u) + d(v)] < \sum_{u \sim v} (m+1)$$

i. e.,

$$M_1(G) < m(m+1) \ , \ \text{contradiction.}$$

From Eq. (1) we conclude that each edge $\{u,v\}$ of a graph G with $n > 3$ vertices, satisfying the relation $M_1(G) = m(m+1)$, has exactly an endpoint that is adjacent to $m-1$ (or $n-2$) pendent edges. Therefore, $G \cong K_{1,n-1}$. □

Lemma 2. If G is a connected (n,m) graph with $D = 1$, then $M_1(G) = n(n-1)^2$.

Proof. The unique connected n-vetrex graph with diameter 1 is the complete graph K_n. Each of its vertices is of degree $n-1$. □

Lemma 3. Let $G = (V,E)$ be a connected (n,m) graph with girth $g(G) \geq 4$. Then $M_1(G) \leq m^2$. Equality holds if and only if $G \cong C_4$.

Proof. Since $g(G) \geq 4$, the graph G must contain an r-membered cycle C_r , $r \geq 4$. For any $\{u,v\} \in E$, $d(u) + d(v) \neq m+1$, i. e., $d(u) + d(v) \leq m$. Then

$$M_1(G) = \sum_{u \sim v} [d(u) + d(v)] \leq \sum_{u \sim v} m = m^2 \ .$$

Assume that $M_1(G) = m^2$. Then $d(u) + d(v) = m$ holds for any $\{u,v\} \in E$. This implies that the only graph with $g(G) \geq 4$ and the property $M_1(G) = m^2$ is C_4. □

Theorem 1. Let G be an (n,m) graph with diameter D. Then

$$\begin{aligned} M_1(G) &= n(n-1)^2 \qquad \text{if} \quad D = 1 \quad \text{(Lemma 2)} \\ M_1(G) &\leq m^2 - m(D-3) + (D-2) \qquad \text{if} \quad D > 1 \ . \end{aligned} \tag{2}$$

If $D = 2$ then equality in (2) holds if only if either $G \cong K_{1,n-1}$ or $G \cong K_3$. If $D \geq 3$ then equality in (2) holds if and only if $G \cong P_{D+1}$ (the path of order $D+1$).

Proof. We need to consider only the case $D(G) > 1$. If $D(G) > 1$ then there exists a path P of length D in G. Let $P = u_0, u_1, u_2, \ldots, u_{D-1}, u_D$, where $u_i \in V(G)$, $i = 1, 2, \ldots, D$. Then

$$\begin{aligned} d(u_0) + d(u_1) &\leq m - (D-3) \\ d(u_i) + d(u_{i+1}) &\leq m - (D-4) \quad \text{for } i = 1, 2, \ldots, D-2 \\ d(u_{D-1}) + d(u_D) &\leq m - (D-3) \ . \end{aligned}$$

If $V(G) \setminus V(P) \neq \emptyset$, then for any two vertices $u, v \in V(G)$, of which at least one belongs to $V(G) \setminus V(P)$, the condition $d(u) + d(v) \leq m - (D-3)$ is satisfied. Consequently,

$$\begin{aligned} \sum_{u \sim v} [d(u) + d(v)] &\leq \sum_{u \sim v} [m - (D-3)] + (D-2) \\ M_1(G) &\leq m^2 - (D-3)\, m + (D-2) \ . \end{aligned}$$

Equality in (2) will hold if and only if all the above relations are equalities. It is not difficult to check that for $D = 2$ this happens if either $G \cong K_{1,n-1}$ or $G \cong K_3$, whereas for $D \geq 3$, if $G \cong P_{D+1}$. $\Box$

Remark 1. The bound given in Theorem 1 is the best possible in its class. When $D = 2$, then $M_1 \leq m^2 + m$. When $D = 3$, then $M_1 \leq m^2 + 1$. When $D = 4$, then $M_1 \leq m^2 - m + 2$.

Remark 2. If we consider bounds for M_1 in terms of the girth of G, then for $g(G) \leq 3$ (including the case when the graph is acyclic), the bound stated in Theorem 1 is applicable. When $g(G) \geq 4$, then by Lemma 3, $M_1 \leq m^2$.

Remark 3. In fact, the condition $g(G) \geq 4$ in Lemma 3 can be replaced by the condition that G contains an elemental circuit of length at least 4.

UPPER BOUNDS FOR M_2

The following upper bounds for M_2 have been obtained.

Theorem E [13]. Let G be an (n,m) graph. Then

$$M_2(G) \leq m\left(\sqrt{2m+\frac{1}{4}}-\frac{1}{2}\right)^2$$

with equality holding if and only if G is the union of a complete graph and isolated vertices.

Theorem F [8]. Let G be an (n,m) graph with minimal vertex degree δ. Then

$$M_2(G) \leq 2\,m^2 - (n-1)\,m\,\delta + \frac{1}{2}\,(\delta-1)\,M_1(G)\ .$$

Theorem G [11]. Let G be an (n,m) graph and let λ_1 be the greatest Laplacian eigenvalue. Then

$$M_2(G) \leq \frac{\lambda_1}{2}\ M_1(G) \leq \frac{n}{2}\,(2m-n+1)^{3/2}\ .$$

By Theorems F, G, and 1, we have:

Theorem 2. Let G be a connected (n,m) graph with diameter $D > 1$. Then

$$\begin{aligned} M_2 &\leq 2\,m^2 - (n-1)\,m\,\delta + \frac{1}{2}\,(\delta-1)\,[m^2 - m(D-3) + (D-2)] \\ M_2 &\leq \frac{1}{2}\,[m^2 - m(D-3) + (D-2)]\,\sqrt{2m-n+1}\ . \end{aligned}$$

Examples show that the bounds in Theorem 2 are better than those in Theorems E and G.

In what follows we derive a few relations connecting the second Zagreb index of a graph G and of its complement $\overline{G}$.

Lemma 4. Let $\overline{G}$ be the complement of the (n,m) graph G. Then

$$M_1(G) - M_1(\overline{G}) = 2(n-1)(m-\overline{m}) \tag{3}$$

where $\overline{m} = \binom{n}{2} - m$ is the number of edges of $\overline{G}$.

Proof.

$$\begin{aligned} M_1(G) + M_1(\overline{G}) &= \sum_{i=1}^{n} d_i^2 + \sum_{i=1}^{n} (n-1-d_i)^2 \\ &= \sum_{i=1}^{n} \left[d_i^2 + (n-1)^2 - 2(n-1)\, d_i + d_i^2 \right] \\ &= 2 \sum_{i=1}^{n} d_i^2 + n(n-1)^2 - 2(n-1) \cdot 2\, m \\ &= 2\, M_1(G) + n(n-1)^2 - 4\, m\, (n-1) \ . \end{aligned}$$

Simplifying, we arrive at Eq. (3). □

Lemma 5. Let the notation be the same as in Lemma 4. Then

$$\frac{1}{2} M_1(G) - (n-1)\, M_1(\overline{G}) + M_2(G) + M_2(\overline{G}) = 2\, m^2 - (n-1)^2\, \overline{m} \ . \qquad (4)$$

Proof. Denote by $\overline{d_i}$ the degree of the vertex i in $\overline{G}$.

$$\begin{aligned} M_1(G) &= \sum_{i=1}^{n} d_i^2 = \left(\sum_{i=1}^{n} d_i \right)^2 - 2 \sum_{\substack{i,j \in V \\ i \neq j}} d_i\, d_j \\ &= 4\, m^2 - 2 \left(\sum_{i \sim j} d_i\, d_j + \sum_{i \not\sim j} d_i\, d_j \right) \\ &= 4\, m^2 - 2 \left[M_2(G) + \sum_{i \not\sim j} \left(n-1-\overline{d_i}\right) \left(n-1-\overline{d_j}\right) \right] \\ &= 4\, m^2 - 2 \left[M_2(G) + \sum_{i \not\sim j} (n-1)^2 - (n-1) \sum_{i \not\sim j} (\overline{d_i} + \overline{d_j}) + \sum_{i \not\sim j} \overline{d_i}\, \overline{d_j} \right] \\ &= 4\, m^2 - 2\, M_2(G) - 2(n-1)^2 \left[\binom{n}{2} - m \right] + 2(n-1)\, M_1(\overline{G}) - 2\, M_2(\overline{G}) \ . \end{aligned}$$

Eq. (4) follows. □

Combining the identities (3) and (4) we obtain:

$$M_2(G) = 2\, m^2 - (n-1)^2\, (2\, m - \overline{m}) + \left(n - \frac{3}{2} \right) M_1(G) - M_2(\overline{G})$$

which together with Theorem 1 and the obvious relation $M_2(\overline{G}) \geq \overline{m}$ yields a further upper bound for M_2:

Theorem 3. Let G be an (n,m) graph, $n > 1$, with diameter D. Then

$$\begin{aligned} M_2(G) &\leq 2\,m^2 - (n-1)^2\,(2m - \overline{m}) \\ &+ \frac{1}{2}\,(2n-3)[m^2 - m(D-3) + (D-2)] - \overline{m}\,. \end{aligned}$$

In spite of its neat form, the inequality given in Theorem 3 is significantly weaker than those in Theorem 2. We stated it just because of completeness.

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