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ZAGREB INDICES

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Abstract

For a (molecular) graph, the first Zagreb index M_1 is equal to the sum of the squares of the degrees of the vertices, and the second Zagreb index M_2 is equal to the sum of the products of the degrees of pairs of adjacent vertices. We provide upper bounds for the Zagreb indices M_1 and M_2 of a graph, especially for triangle-free graphs, in terms of the number of vertices and the number of edges, and determine the graphs for which the bounds are attained.

INTRODUCTION

Let G be a graph without loops and multiple edges. The first Zagreb index M_1 and the second Zagreb index M_2 of G are defined as follows:

$$M_1 = M_1(G) = \sum_{\text{vertices}} (d_u)^2$$

$$M_2 = M_2(G) = \sum_{\text{edges}} d_u d_v$$

where d_u is the degree of vertex u.

The Zagreb indices M_1 and M_2 were introduced in [1] and elaborated in [2]. The main properties of M_1 and M_2 were summarized in [3] and [4] recently. These indices reflect the extent of branching of the molecular carbon-atom skeleton, and can thus be viewed as molecular structure-descriptors [5, 6].

Let G be a graph with vertex set $V = \{v_1, \ldots, v_n\}$ and m edges. For any vertex v, $\Gamma(v)$ denotes the set of the first neighbors of v. For each i, $1 \leq i \leq n$, set $d_i = d_{v_i}$ and $F(v_i) = V - \Gamma(v_i) \cup \{v_i\}$. Thus $F(v_i)$ is the set of vertices far from v_i, at distance at least 2. Write e_i for the number of edges connecting vertices in $\Gamma(v_i)$ to vertices in $F(v_i)$ and f_i for the number of edges connecting vertices in $F(v_i)$. Note that

$$\sum_{v_j \in \Gamma(v_i)} d_j = 2m - d_i - e_i - 2f_i \,.$$

Consequently

$$\begin{aligned} M_1(G) &= \textstyle\sum_{i=1}^n \sum_{v_j \in \Gamma(v_i)} d_j \\ &= \textstyle\sum_{i=1}^n (2m - d_i - e_i - 2f_i) \\ &= 2mn - \textstyle\sum_{i=1}^n (d_i + e_i + 2f_i) \end{aligned} \tag{1}$$

and

$$\begin{aligned} M_2(G) &= \tfrac{1}{2} \textstyle\sum_{i=1}^n d_i \sum_{v_j \in \Gamma(v_i)} d_j \\ &= \tfrac{1}{2} \textstyle\sum_{i=1}^n d_i (2m - d_i - e_i - 2f_i) \\ &= 2m^2 - \tfrac{1}{2} \textstyle\sum_{i=1}^n d_i (d_i + e_i + 2f_i) \,. \end{aligned} \tag{2}$$

In this article, we provide upper bounds for the Zagreb indices M_1 and M_2 of a graph, especially of triangle-free graphs, in terms of the number of vertices and the number of edges, and determine the graphs for which the bounds are attained.

UPPER BOUNDS FOR M_1

Let m be the number of edges of a graph G. A very simple upper bound for M_1 is [7]

$$M_1(G) \leq m(m+1) \,.$$

Clearly this bound can be attained, for example, for the star $K_{1,n-1}$. Recall that Das [7], Caen [8] and Li and Pan [9] have obtained the following:

Theorem 1. [7, 8, 9] *Let G be a graph with n vertices and $m > 0$ edges. Then*

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

and equality holds if and only if G is K_n, $K_{1,n-1}$ or $K_1 \cup K_{n-1}$.

Knowing the value of the maximum degree, the bound in Theorem 1 can be sharpened [7]. When we know the value of the minimum degree, we have

Theorem 2. *Let G be a graph with n vertices, m edges and minimum degree δ. Then*

$$M_1(G) \le n(2m-\delta n) + \frac{n}{2}\left(\delta^2 + 1 + (\delta-1)\sqrt{(\delta+1)^2 + 4(2m-\delta n)}\right)$$

and equality holds if and only if G is a regular graph or $K_{1,n-1}$.

Proof. It is known that [10] $M_1(G) \le n\lambda_1^2$ and equality holds if and only if G is a regular graph or a bipartite semiregular graph, where λ_1 is the largest eigenvalue of the adjacency matrix of G. From [11],

$$\lambda_1 \le \frac{1}{2}\left(\delta - 1 + \sqrt{(\delta+1)^2 + 4(2m-\delta n)}\right)$$

and equality holds if and only if in one component of G each vertex is either of degree δ or adjacent to all other vertices, and all other components are regular with degree δ. Now the result follows easily. □

Remark 3. Let G be a graph with n vertices and m edges and without isolated vertices. Since $2m \le n(n-1)$,

$$\frac{1}{2}\left(x - 1 + \sqrt{(x+1)^2 + 4(2m-xn)}\right)$$

is a decreasing function of x for $1 \le x \le n-1$. By Theorem 2, we know that

$$M_1(G) \le n(2m-n+1)$$

and equality holds if and only if G is K_n, $K_{1,n-1}$ or mK_2.

Remark 4. Let G be a graph with n vertices and m edges. Define d, t by $m = \binom{d}{2} + t$, $0 \le t < d$. Let C_n^m be the graph obtained from K_d by adding a vertex of degree t and $n-d-1$ isolated vertices. Let S_n^m be the complement of $C_n^{\binom{n}{2}-m}$. Then an upper bound for $M_1(G)$ is already known [12]: $M_1(G) \le M_1(C_n^m) = t^2 + t(d-t)^2 + (d-t)(d-t-1)^2$ if $m > \frac{1}{2}\binom{n}{2} + \frac{n}{2}$, and $M_1(G) \le M_1(S_n^m)$ if $m < \frac{1}{2}\binom{n}{2} - \frac{n}{2}$.

Theorem 5. *Let G be a triangle-free graph with n vertices and $m > 0$ edges. Then $M_1(G) \le mn$ and equality holds if and only if G is a complete bipartite graph.*

Proof. Note that since G is triangle-free, we have

$$d_i + e_i + f_i = m\,.$$

By (1), we have

$$M_1(G) = 2mn - \sum_{i=1}^{n}(d_i + e_i + 2f_i) \le 2mn - mn = mn\,.$$

If $M_1(G) = mn$, we must have $f_i = 0$ for all i. Hence G is a bipartite complete graph. It is immediate that if $G = K_{r,n-r}$ with $1 \le r \le n/2$ then we do have $M_1(G) = mn$. □

Remark 6. Let G be a triangle-free graph with n vertices. Let m be the number of edges of G. By Turán's theorem, $m \le \lfloor n^2/4 \rfloor$ and equality holds if and only if $G = K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$. By Theorem 5,

$$M_1(G) \le n \left\lfloor n^2/4 \right\rfloor$$

and equality holds if and only if $G = K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$. If G is a tree with n vertices, then by Theorem 1, 2, or 5,

$$M_1(G) \le n(n-1)$$

and equality holds if and only if $G = K_{1,n-1}$ (see also [4]).

UPPER BOUNDS FOR M_2

Now we consider upper bounds for M_2. Note that Bollobás and Erdős [13] have proven the following:

Theorem 7. [13] *Let G be a graph with m edges. Then*

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

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

Let G be a graph with n vertices, m edges and minimal degree δ. Then [14] $M_2(G) \le 2m^2 - (n-1)m\delta + \frac{1}{2}(\delta - 1)M_1(G)$.

Theorem 8. *Let G be a graph with n vertices and let λ_1 be the largest eigenvalue of the adjacency matrix of G. Then $M_2(G) \le \lambda_1 M_1(G)/2$ and equality holds if and only if $(d_1, d_2, \ldots, d_n)^T$ is an eigenvector of the adjacency matrix corresponding to λ_1.*

Proof. Let A be the adjacency matrix of G. It is well known that

$$\lambda_1 \ge \frac{x^T A x}{x^T x}$$

with equality if and only if x is an eigenvector of A corresponding to λ_1. Setting $x = (d_1, d_2, \ldots, d_n)^T$, we obtain the desired result. □

From this theorem we can obtain upper bounds for $M_2(G)$ from upper bounds for λ_1 and $M_1(G)$. For example, let G be a graph with n vertices and m edges and without isolated vertices. Then by the proof of Theorem 2 and Remark 3, we have

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

and equality holds if and only if G is K_n or mK_2.

Theorem 9. *Let G be a triangle-free graph with $m > 0$ edges. Then*

$$M_2(G) \leq m^2$$

and equality holds if and only if G is the union of a complete bipartite graph and isolated vertices.

Proof. Note that since G is triangle-free, we have

$$d_i + e_i + f_i = m\,.$$

Consequently by (2)

$$M_2(G) = 2m^2 - \frac{1}{2}\sum_{i=1}^{n} d_i(d_i + e_i + 2f_i) \leq 2m^2 - \frac{1}{2}\sum_{i=1}^{n} d_i m = m^2.$$

If $M_2(G) = m^2$, we must have $f_i = 0$ whenever $d_i > 0$. Hence, G is the union of a complete bipartite graph and isolated vertices. It is immediate that if G is the union of a complete bipartite graph $K_{r,s}$ and isolated vertices then $M_2(G) = r^2s^2 = m^2$. □

Remark 10. Let G be a triangle-free graph with n vertices. Then by Theorem 9,

$$M_2(G) \leq \lfloor n^2/4 \rfloor^2$$

and equality holds if and only if $G = K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$. If G is a tree with n vertices, then by Theorem 9,

$$M_2(G) \leq (n-1)^2$$

and equality holds if and only if $G = K_{1,n-1}$ [14].

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