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A NOTE ON 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 quadrangle-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 simple graph with vertex set $V(G)$ and edge set $E(G)$. For $u \in V(G)$, $\Gamma(u)$ denotes the set of its (first) neighbors in G and the degree of u is $d_u = |\Gamma(u)|$. The *first Zagreb index* M_1 and the *second Zagreb index* M_2 of G are defined as follows:

$$M_1 = M_1(G) = \sum_{u \in V(G)} (d_u)^2$$

$$M_2 = M_2(G) = \sum_{uv \in E(G)} d_u d_v \,.$$

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, 4], and some recent results can be found in

[5–12]. These indices reflect the extent of branching of the molecular carbon atom skeleton, and can thus be viewed as molecular structure-descriptors [13, 14].

In [6] the first author considered upper bounds for the Zagreb indices M_1 and M_2 of triangle-free graphs. We now provide upper bounds for M_1 and M_2 of quadrangle-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

Before we state our first bound, let us slightly redefine a class of graphs usually called *windmills*. For n odd, a windmill W_n is a graph obtained by taking $\frac{n-1}{2}$ triangles all sharing one common vertex. For n even, a windmill W_n is a graph obtained from a windmill W_{n-1} by attaching a pendant vertex to a central vertex of W_{n-1}. In any case, a windmill W_n has n vertices.

For quadrangle-free graphs, we have the following.

Theorem 1. *Let G be a quadrangle-free graph with n vertices and $m > 0$ edges. Let*

$$even(n) = \begin{cases} 1, & n \text{ is even,} \\ 0, & n \text{ is odd.} \end{cases}$$

Then

$$M_1(G) \leq n(n-1) + 2m - 2\,even(n) \tag{1}$$

with equality if and only if G is isomorphic to a windmill W_n.

Proof. Since G is quadrangle-free, we have $|\Gamma(x) \cap \Gamma(y)| \leq 1$ for any two distinct vertices x and y of G. For any $u \in V(G)$, let

$$A_u = \{\{x, y\} : \Gamma(x) \cap \Gamma(y) = \{u\}, x, y \in V(G), x \neq y\}.$$

Then $A_u \cap A_v = \emptyset$ if $u \neq v$. It follows that

$$\sum_{u \in V(G)} \binom{d_u}{2} = \sum_{u \in V(G)} |A_u| \leq \binom{n}{2},$$

which proves (1) when n is odd. In such case, equality holds if and only if $|\Gamma(x) \cap \Gamma(y)| = 1$ for any two distinct vertices x and y of G. By the Friendship Theorem (which characterizes graphs with this property; see, e.g., [15, 16]), G is isomorphic to a windmill W_n in this case.

If n is even, then there is at least one pair $\{x', y'\}$ of vertices with $|\Gamma(x') \cap \Gamma(y')| = 0$, so that

$$\sum_{u \in V(G)} \binom{d_u}{2} = \sum_{u \in V(G)} |A_u| \leq \binom{n}{2} - 1,$$

and (1) follows again. The equality holds if and only if $|\Gamma(x) \cap \Gamma(y)| = 1$ for any pair of vertices $\{x, y\} \neq \{x', y'\}$. Such graphs are characterized by the following lemma.

Lemma 2. *If a graph G with n vertices contains a pair of vertices $\{x', y'\}$ without a common neighbor, while every other pair of vertices has exactly one common neighbor, then n is even and G is isomorphic to a windmill W_n.*

Proof of Lemma 2. Let us classify the vertices of $G - x' - y'$ into the following disjoint sets:

- set I is formed by vertices adjacent to x';
- set J is formed by vertices adjacent to y';
- set K is formed by the remaining vertices.

Each pair of vertices from I has x' as a common neighbor, so no two vertices from I are adjacent to the same vertex $\neq x'$. Moreover, each vertex from I and x' have exactly one common neighbor, which, being a neighbor of x', must belong to I. Thus, we may conclude that the subgraph induced by vertices in I is isomorphic to aK_2 for some $a \in \mathbf{N}$, yielding $|I| = 2a$. Similarly, the subgraph induced by vertices in J is isomorphic to bK_2 for some $b \in \mathbf{N}$ and $|J| = 2b$.

Each vertex from K must have a common neighbor with x', so it has exactly one neighbor in I. Also, it must have a common neighbor with y', so it has exactly one neighbor in J. Thus, vertices from K may be indexed by pairs $(i, j) \in I \times J$ in such a way that a vertex $k_{i,j}$ is adjacent to $i \in I$ and $j \in J$. Moreover, $k_{i,j}$ is the common neighbor of i and j, and so there may not be two vertices from K indexed by the same pair (i, j).

Suppose first that both I and J are nonempty.

Suppose now that x' and y' are not adjacent. Consider an arbitrary vertex $i \in I$. It has exactly one common neighbor with y', and let it be $j \in J$. So, vertices i and j are adjacent, while i is not adjacent to any other vertex from J. Consider now vertices of the form $k_{ij'}$, $j' \neq j$. From above, there are $2b - 1$ such vertices. Fix $p \in J \setminus \{j\}$. Vertex k_{ip} must have a common neighbor with i, and that common neighbor does not belong to J. Thus, it has to belong to K. But i is adjacent only to vertices of the form $k_{ij'}$. Suppose that common neighbor is k_{iq}. It cannot be $q = j$, as then i and k_{ij} would have two common neighbors: j and k_{ip}! So, every vertex of the form k_{ip}, $p \neq j$, is adjacent to exactly one other vertex of the form k_{iq}, $q \neq j$, yielding that the subgraph induced by vertices $k_{ij'}$, $j' \neq j$, is isomorphic to cK_2 for some $c \in \mathbf{N}$. From here we conclude that there are $2c$ vertices of the form $k_{ij'}$, $j' \in J$. However, this is a contradiction, as the equality $2b - 1 = 2c$ cannot hold in $\mathbf{N}$.

Suppose now that x' and y' are adjacent. Each vertex from I and y' have x' already as a common neighbor, so no vertex from I can be adjacent to any vertex from J. Consider an arbitrary vertex $k_{ij} \in K$. It has exactly one common neighbor with i, which, being a neighbor of i, must also be of the form $k_{ij'}$, $j' \in J$. Consider now vertices $i' \in I \setminus \{i\}$. If i and i' are adjacent, then i is a common neighbor of i' and k_{ij}, and in such case, k_{ij} is not adjacent to any vertex of the form $k_{i'j'}$, $j' \in J$. If i and i' are not adjacent, then k_{ij} is adjacent to exactly one vertex of the form $k_{i'j'}$, $j' \in J$. Altogether, we conclude that the degree of k_{ij} within K is $2a - 1$. If we exchange the roles of I and J in the above analysis, then it yields that the degree of k_{ij} within K is $2b - 1$, i.e., it must hold that

$$a = b\,.$$

Therefore, set K contains $4a^2$ vertices.

Next, vertex k_{ij} has i as a common neighbor with vertices of the form $k_{ij'}$, $j' \in J \setminus \{j\}$, and it has j as a common neighbor with vertices of the form $k_{i'j}$, $i' \in I \setminus \{i\}$. Vertex k_{ij} has a common neighbor within K with the remaining $4a^2 - 4a + 1 = (2a - 1)^2$ vertices from K. We may, therefore, conclude that there are

$$\frac{4a^2(2a-1)^2}{2} = 2a^2(2a-1)^2$$

pairs of vertices from K that have a common neighbor within K.

On the other hand, each vertex from K has degree $2a-1$ within K and so it is a common neighbor for $\binom{2a-1}{2}$ pairs of vertices from K. Altogether, all vertices from K serve as a common neighbor for

$$4a^2\binom{2a-1}{2} = 2a^2(2a-1)(2a-2)$$

pairs of vertices from K. As

$$2a^2(2a-1)(2a-2) < 2a^2(2a-1)^2\,,$$

we conclude that not every pair of vertices from K can have a common neighbor, which is a contradiction.

From the above contradictions, we conclude that the only possible case is that one of the sets I and J is empty. Without loss of generality, suppose that J is empty. Then K must also be empty. As we already know that the subgraph induced by vertices in I is isomorphic to aK_2, we can now finally see that the whole graph G is isomorphic to a windmill W_{2a+2} and that $n = 2a+2$ is even. □

Remark 3. Let G be a $K_{2,r}$-free graph with n vertices and m edges, where $r \geq 2$. Then by similar arguments as those in the proof of Theorem 1,

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

with equality if and only if $|\Gamma(x) \cap \Gamma(y)| = r-1$ for any two distinct vertices x and y of G.

Remark 4. Let G be a graph with m edges and girth r. Then for any $uv \in E(G)$, $d_u + d_v \leq m - r + 4$ with equality if and only if uv lies on a cycle with r vertices and every edge outside this cycle (if it exists) is incident with u or v. So

$$M_1(G) = \sum_{uv\in E(G)} (d_u + d_v) \leq m(m-r+4)$$

with equality if and only if G is a cycle with $m = r$ vertices.

Further, we consider triangle- and quadrangle-free graphs. Recall [17] that the Moore graphs of diameter 2 (regular graph of diameter 2 and girth 5) are pentagon, Petersen graph, Hoffman-Singleton graph, and possibly a 57-regular graph with 3250 vertices (its existence is still an open problem). They are $\sqrt{n-1}$-regular graphs with $n = 5, 10, 50$, and possibly $n = 3250$ vertices, respectively.

Theorem 5. *Let G be a triangle- and quadrangle-free graph with $n > 1$ vertices. Then*

$$M_1(G) \leq n(n-1) \tag{2}$$

with equality if and only if G is a star $K_{1,n-1}$ or a Moore graph of diameter 2.

Proof. The statement is trivial for $n = 2$. Suppose that $n \geq 3$, and let u be an arbitrary vertex of G. Let us bound $\sum\limits_{v\in\Gamma(u)} d_v$, which counts the number of edges originating from vertices in $\Gamma(u)$. First, there are d_u edges leading to u. Then, as G is quadrangle-free, a vertex from $V(G) \setminus (\{u\} \cup \Gamma(u))$ may be adjacent to at most one vertex from $\Gamma(u)$. Thus, there are at most

$n - d_u - 1$ edges connecting a vertex from $V(G) \setminus (\{u\} \cup \Gamma(u))$ and a vertex from $\Gamma(u)$. Finally, since G is triangle-free, $\Gamma(u)$ is an independent set. Thus,

$$\sum_{v \in \Gamma(u)} d_v \le d_u + (n - d_u - 1) = n - 1$$

and if equality holds, then $\bigcup_{v \in \Gamma(u)} \Gamma(v) = V(G)$, which implies that the distance between u and any other vertex of G is at most 2. Thus

$$M_1(G) = \sum_{u \in V(G)} \sum_{v \in \Gamma(u)} d_v \le \sum_{u \in V(G)} (n-1) = n(n-1)\,.$$

This proves (2).

Now suppose that equality holds in (2). Then $\sum_{v \in \Gamma(u)} d_v = n - 1$ for every $u \in V(G)$ and so the diameter of G is 2. Bondy et al. [18] had proved that a quadrangle-free graph with n vertices and diameter 2 is a graph of maximum vertex degree $n-1$, or a Moore graph, or a polarity graph. However, a polarity graph is not triangle-free (see [18]). It follows that $G \cong K_{1,n-1}$ or G is a Moore graph.

Conversely, if $G \cong K_{1,n-1}$ or G is a Moore graph of diameter 2, then it is immediate to check that (2) is an equality. $\square$

UPPER BOUNDS FOR M_2

Let G be a graph. From the definition of M_2, it follows that

$$M_2(G) = \frac{1}{2} \sum_{u \in V(G)} d_u \sum_{v \in \Gamma(u)} d_v\,.$$

We will use this observation in the proof of the following theorems.

Theorem 6. *Let G be a quadrangle-free graph with n vertices and $m > 0$ edges. Then*

$$M_2(G) \le mn + \binom{n}{2} - even(n) \tag{3}$$

with equality if and only if G is isomorphic to a windmill W_n for odd n.

Proof. The statement is trivial for $n = 2$. Suppose that $n \ge 3$. Since G is quadrangle-free, any two vertices from $\Gamma(u)$ have distinct neighbors other than u. Moreover, note that the subgraph $G(\Gamma(u))$ induced by vertices in $\Gamma(u)$ may not contain path P_3 as a subgraph, as P_3 together with u forms a quadrangle in G. So, $G(\Gamma(u))$ has maximum degree at most 1, and as a consequence, at most $\left\lfloor \frac{d_u}{2} \right\rfloor$ edges. Hence, as every of these edges is counted twice in $\sum_{v \in \Gamma(u)} d_v$, we have that $\sum_{v \in \Gamma(u)} d_v \le n - 1 + 2 \left\lfloor \frac{d_u}{2} \right\rfloor$. Thus

$$M_2(G) \;=\; \frac{1}{2} \sum_{u \in V(G)} d_u \sum_{v \in \Gamma(u)} d_v$$

$$
\begin{aligned}
&\le \frac{1}{2}\sum_{u\in V(G)} d_u\left(n-1+2\left\lfloor\frac{d_u}{2}\right\rfloor\right)\\
&= \frac{n-1}{2}\sum_{u\in V(G)} d_u + \sum_{u\in V(G)} d_u\left\lfloor\frac{d_u}{2}\right\rfloor\\
&\le m(n-1)+\frac{1}{2}M_1(G)\\
&\le mn+\frac{1}{2}n(n-1)-even(n)\,,
\end{aligned}
$$

where the last inequality follows from Theorem 1.

In order for equality to hold, we must have that G is a windmill W_n with even vertex degrees, i.e., that n is odd. On the other hand, it is straightforward to check that equality is indeed satisfied for such graphs. □

Theorem 7. *Let G be a triangle- and quadrangle-free graph with n vertices and $m > 0$ edges. Then*

$$M_2(G) \le m(n-1) \tag{4}$$

with equality if and only if G is a star $K_{1,n-1}$ or a Moore graph of diameter 2.

Proof. The statement is trivial for $n = 2$. Suppose that $n \ge 3$. Since G is triangle- and quadrangle-free, we have $\sum\limits_{v\in\Gamma(u)} d_v \le n-1$ for any $u \in V(G)$ and if equality holds, then the distance between u and any other vertex of G is at most 2. Thus

$$M_2(G) = \frac{1}{2}\sum_{u\in V(G)} d_u \sum_{v\in\Gamma(u)} d_v \le \frac{1}{2}\sum_{u\in V(G)} d_u(n-1) = m(n-1)\,.$$

This proves (4).

Now suppose that equality holds in (4). By the arguments as in the proof of Theorem 5, $G \cong K_{1,n-1}$ or G is a Moore graph of diameter 2.

Conversely, if $G \cong K_{1,n-1}$ or G is a Moore graph of diameter 2, then it is easy to check that (4) is an equality. □

Besides n and m, the upper bounds in the next two theorems depend also on the minimum vertex degree δ.

Theorem 8. *Let G be a quadrangle-free graph with n vertices, m edges and minimum vertex degree $\delta \ge 1$. Then*

$$M_2(G) \le 2m^2-(n-1)m\delta+(\delta-1)\left[\binom{n}{2}+m\right] \tag{5}$$

with equality if and only if G is isomorphic to a windmill W_n for odd n, or $\frac{n}{2}K_2$ for even n, or a star $K_{1,n-1}$.

Proof. This bound follows from a different estimate of $\sum\limits_{v\in\Gamma(u)} d_v$. Namely, for all $u \in V(G)$ it holds that

$$\sum_{v\in\Gamma(u)} d_v \le 2m-d_u-(n-1-d_u)\delta\,,$$

which is just a rewriting of an obvious inequality

$$2m = \sum_{u\in V(G)} d_u = d_u + \sum_{v\in\Gamma(u)} d_v + \sum_{w\in V(G)\setminus(\{u\}\cup\Gamma(u))} d_w \geq d_u + \sum_{v\in\Gamma(u)} d_v + (n-1-d_u)\delta\,.$$

Note that equality holds above if and only if either $d_u = n-1$ or all vertices not adjacent to u are of degree δ. Then

$$\begin{aligned} M_2(G) &= \frac{1}{2}\sum_{u\in V(G)} d_u \sum_{v\in\Gamma(u)} d_v \\ &\leq \frac{1}{2}\sum_{u\in V(G)} d_u[2m - d_u - (n-1-d_u)\delta] && (6) \\ &= 2m^2 - (n-1)m\delta + \frac{1}{2}(\delta-1)M_1(G) \\ &\leq 2m^2 - (n-1)m\delta + \frac{1}{2}(\delta-1)[n(n-1)+2m]\,. && (7) \end{aligned}$$

This proves (5).

Now suppose that equality holds in (5). Then all inequalities above become equalities. From (6) we have for every vertex u either $d_u = n-1$ or all vertices not adjacent to u are of degree δ. If $\delta > 1$, then from (7) and Theorem 1 it follows that G is isomorphic to a windmill W_n for some odd n. If $\delta = 1$, then for any vertex u with $d_u = 1$, all vertices not adjacent to u are of degree 1, and so $G \cong \frac{n}{2}K_2$ for even n or $G \cong K_{1,n-1}$.

Conversely, if G is isomorphic to a windmill W_n for odd n, or $\frac{n}{2}K_2$ for even n, or a star $K_{1,n-1}$, then it is easy to check that (5) is an equality. □

Similarly, we have

Theorem 9. *Let G be a triangle- and quadrangle-free graph with n vertices, m edges and minimum vertex degree $\delta \geq 1$. Then*

$$M_2(G) \leq 2m^2 - (n-1)m\delta + (\delta-1)\binom{n}{2} \tag{8}$$

with equality if and only if G is a star $K_{1,n-1}$, or $\frac{n}{2}K_2$ for even n, or G is a Moore graph of diameter 2.

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